

A graph-theoretical approach for the computation of connected iso-surfaces based on volumetric data

Abdulaziz Ali and Dieter Bothe

Mathematical Modeling and Analysis
Center of Smart Interfaces
TU Darmstadt
Alarich-Weiss-Str. 10
64287 Darmstadt
Germany

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Abstract

The existing combinatorial methods for iso-surface computation are efficient for pure visualization purposes, but it is known that the resulting iso-surfaces can have holes, and topological problems like missing or wrong connectivity can appear. To avoid such problems, we introduce a graph-theoretical method for the computation of iso-surfaces on cuboid meshes in \mathbb{R}^3 . The method for the generation of iso-surfaces employs labeled cuboid graphs $G(V, E, \mathcal{F})$ such that V is the set of vertices of a cuboid $C \subset \mathbb{R}^3$, E is the set of edges of C and $\mathcal{F} : V \rightarrow [0, 1]$. The nodes of G are weighted by the values of \mathcal{F} which represents the volumetric information, e.g. from a Volume of Fluid method. Using a given iso-level $c \in (0, 1)$, we first obtain all iso-points, i.e. points where the value c is attained by the edge-interpolated \mathcal{F} -field. The iso-surface is then built from iso-elements which are composed of triangles and are such that their polygonal boundary has only iso-points as vertices. All vertices lie on the faces of a single mesh cell.

We give a proof that the generated iso-surface is connected up to the boundary of the domain and it can be decomposed into different oriented components. Two different components may have discrete points or line segments in common. The graph-theoretical method for the computation of iso-surfaces developed in this paper enables to recover local information of the iso-surface that can be used e.g. to compute discrete mean curvature and to solve surface PDEs. Concerning the computational effort, the resulting algorithm is as efficient as existing combinatorial methods.

Keywords: connected iso-surface, iso-surface topology, iso-path, surface pseudo-normal.

1 Introduction

An iso-surface is a level set of a continuous function whose domain is, in the considered case, \mathbb{R}^3 . Iso-surfaces are for example used to visualize scalar volume data processed in medicine, computational fluid dynamics (CFD), geophysics, and chemistry. In medical imaging, by applying X-ray computed tomography (CT) one obtains volume data which can be used to detect bones, tumors and cancer. In two-fluid systems, the Volume of Fluid (VOF) method provides VOF-data which implicitly describes the interface between the fluids.

The Marching Cubes method [7] is a well known method for volume visualization. It is a combinatorial and not a graph-theoretical method, being based on the tabulation of 256 different configurations. This set of possible configurations is not complete and, hence, resulting iso-surfaces can have holes. More generally, it is known that commonly employed iso-surface algorithms can lead to surfaces with wrong connectivities and holes; see [4] and further references therein. While this may not be an issue in a pure visualization context, it is a severe problem if surface transport equations are to be solved, like surfactant transport on a fluid surface [2]. Other works like [9] and [3] resolve the ambiguity in Marching Cubes. In [6], a topological approach for the computation of iso-surfaces is given, some geometrical properties of the iso-surface are derived and an algorithm for the computation of iso-surfaces is given. But there are still configurations which are not covered by [9] as well as by [6]. For example configurations in which an iso-surface only touches one or more vertices of a cuboid are not investigated in [3], [6] and [9].

The present work, we introduce a novel graph-theoretical method for the generation of iso-surfaces. We will show that the generated iso-surface is connected up to the boundary of the domain and it can be decomposed into different oriented components. Two different components may have discrete points or line segments as an intersection. If two different components have common points or line segments, then each single component can be identified and computed as if they are disjoint. This decomposition of iso-surfaces into oriented components can be used e.g. to compute discrete mean curvature and to solve surface PDEs for instance by means of a Finite Area method.

Our graph-theoretical approach employs labeled cuboid graphs. A labeled cuboid graph is denoted by $G(V, E, \mathcal{F})$ such that V is the set of vertices of a cuboid $C \subset \mathbb{R}^3$, E is the set of edges of C and $\mathcal{F} : V \rightarrow [0, 1]$. The nodes of G are weighted by the values of \mathcal{F} and the weights lie in $[0, 1]$. Using a given iso-level $c \in (0, 1)$, we interpolate on each edge of the graph to get all points, where the value c is attained. We call such a point on an edge of G , where the interpolated values equals c , an iso-point if one of the edge end points has a label greater than c and the other one less than or equal to

c. From this we get a piece of iso-surface whose boundary is a polygon such that its vertices are iso-points and each of the edges lies on a face of C . We call such an iso-surface piece an iso-element, its boundary an iso-path and each of the edges of the iso-path an iso-line. To compute the iso-element we use a center point $P \in \mathbb{R}^3$ which is the arithmetic mean of the corresponding iso-points. Then the iso-element is defined as the union of all triangles spanned by an iso-line edge and the vertex P . Each of the sketches (a) to (d) of Figure 1 shows an iso-element of a labeled cuboid graph. Sketch (a) has a triangular iso-element. Sketches (b) to (d) of Figure 1 have iso-elements such that the iso-paths may not lie on a common plane.

The iso-elements described above result from iso-paths which run on the faces of a single graph $G(V, E, \mathcal{F})$. Besides this, iso-elements can also occur from two neighboring graphs in which case they lie on their common face. This special case is of fundamental importance for connectivity of the iso-surface.

Notation 1. Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and $c \in (0, 1)$ be an iso-level. Then we use the symbols $\circ, \ominus, \square, \bullet$ in sketches which illustrate $G(V, E, \mathcal{F})$ as well as subgraphs of it. The symbols are used to characterize the labels of the nodes of G and for interpolated values at points that lie on edges of G . The symbol \ominus correspond to labels less than c . The symbol \bullet correspond to labels greater than c and the symbol \square to labels equal to c . In addition, the symbol \circ correspond to labels less than or equal to c .

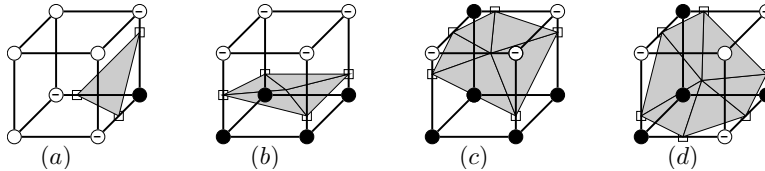


Figure 1: The sketches (a) to (d) show iso-elements of labeled cuboid graphs. Each iso-element is determined by its polygonal boundary, an iso-path.

The iso-surface construction algorithms known so far do not yield in a simple way the local information of the iso-surface such as neighborhood relations at common points or edges of two or more iso-elements. Such topological information is required to compute discrete mean curvature and to solve PDEs on an iso-surface. Hence, the development of a new iso-surface computation method which provides a decomposition of the iso-surface into connected components is required. We achieve this by introducing a purely graph-theoretical method for the computation and decomposition of iso-surfaces. The resulting algorithm is very efficient.

The sketches in Figure 1 show labeled cuboid graphs having one iso-path. But a labeled cuboid graph can have more than one iso-path and

hence more than one iso-element. The sketches in Figure 2 demonstrate that the number of iso-paths depends on the labels of the graph. These are not meaningless, pathological cases, but they occur naturally in dynamic processes with topological changes such as the crown splash of an impacting droplet considered as an application in Section 5. Therefore, one of the main tasks is to introduce a classification of labeled cuboid graphs according to their subgraphs such that the number of iso-paths in a labeled cuboid graph can be identified. The identification of the number of iso-paths and further analysis of the subgraphs of a labeled cuboid graph is the main part of the present work.

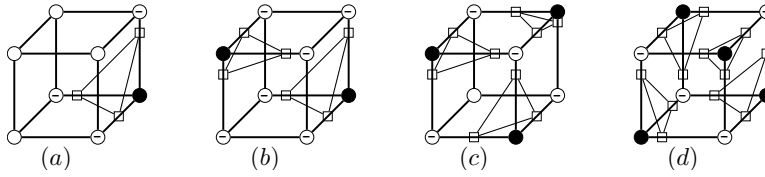


Figure 2: Sketches (a) to (d) show labeled cuboid graphs with one to four distinct iso-paths.

To understand the topology of an iso-surface, we need to investigate pairs of labeled cuboid graphs $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ for a common iso-level $c \in (0, 1)$, where the underlying cuboids C_1 and C_2 , have a common face. Such graphs will be called face-neighbored. If both labeled cuboid graphs have iso-paths with a common iso-line lying on the common face of the cuboids, then they have iso-elements which have a common edge (see Figure 3). In case both end points of the common edge are vertices of the common face then there is a possibility that more than two iso-paths can meet at the common edge. Additionally, if the common iso-line of two iso-paths is a diagonal of a cuboid face, then in each cuboid we can have a maximum of two iso-paths passing through the common edge; hence, it can be a common edge for four different iso-paths. An edge of a cuboid can be a common edge for four distinct cuboids and in each cuboid we can have a maximum of two iso-paths passing through the common edge. Hence, there can be up to eight distinct iso-paths passing through the common edge. All these cases have to be treated for a rigorous iso-surface computation. The sketches in Figure 3 demonstrate two iso-paths of a pair of labeled cuboid graphs with a common edge.

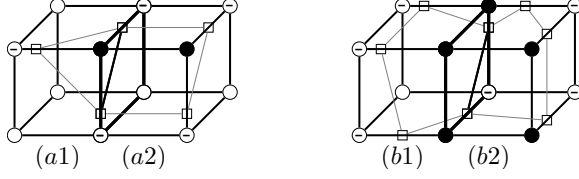


Figure 3: Each pair of sketches (a1), (a2) and (b1), (b2) shows the iso-paths of face-neighbored labeled cuboid graphs. The common face edges in both sketches is bold-framed. Each pair of iso-paths in both sketches above has a common iso-line which is drawn in bold.

An iso-point $P \in \mathbb{R}^3$ of an iso-path can be a common point of 4, 5, 6, 7 or 8 iso-paths. Let P_i for $i = 1, \dots, n$ lie on the i -th iso-path ω_i such that $\overline{PP_i}$ is an iso-line of ω_i . Let P_{c_i} be the center of ω_i . Then we construct a piece of iso-surface region Γ_p using all iso-points P_i and all iso-path centers P_{c_i} and P . Such a region which will be computed in Section 8 is required for computing discrete mean curvature at the iso-point P (see e.g. [8]).

The iso-surface computation algorithm needs a partition \mathcal{T} of a closed polygonal domain $\overline{\Omega} \subset \mathbb{R}^3$ into cuboids such that two cuboids have either a common face or a common vertex or a common edge or they are disjoint. Here, polygonal domain means domain with polygonal boundary. Then, to obtain labeled cuboid graphs, the vertices of each of the cuboids in the partition \mathcal{T} of $\overline{\Omega}$ are labeled with real numbers in $[0, 1]$. The labeled cuboid graphs will be divided into two classes, depending on whether they have a single iso-path or at least two iso-paths (cf., Figure 2). Labeled cuboid graphs of the first class, having only a single iso-path, are called irreducible; members of the other class are called reducible. This classification of labeled cuboid graphs is fundamental for our algorithm.

The algorithm for iso-surface construction uses operations on labeled cuboid graphs such that a reducible labeled cuboid graph $G(V, E, \mathcal{F})$ will be transformed to an irreducible one $G'(V, E, \mathcal{F}')$. Each step in the transformation of G from reducibility to irreducibility gives an iso-element of G . An irreducible labeled cuboid graph finally has a single iso-element. In addition, we can have an iso-path on single faces of a reducible labeled cuboid graph, on which at least two iso-lines lie.

We get the iso-surfaces by collecting all iso-elements of each of the labeled cuboid graphs in \mathcal{T} . The algorithm provides rich local information on the iso-surface like the number of iso-elements with a common edge, or iso-elements with at least one edge of it being an edge of the underlying cuboid net, or at least one edge of the iso-element being a face diagonal of a cuboid. These local information is used for a simple identification of the connected components of the iso-surface.

Another main result of the present work is that the number $n \in \mathbb{N}$ of iso-elements with a common iso-line is an element of $\{2, 4, 6, 8\}$. Hence, the

number of connected components of the iso-surface with a common iso-line may be an element of $\{1, 2, 3, 4\}$. In particular, we will show that triple lines at which three surfaces meet do not occur.

The same principle ideas works to discretization using tetrahedra [1]. It is very likely that the same principle ideas can be adapted to other discretizations (more general polyhedral cells) and also to space dimensions different from 3.

This algorithm for computation of iso-surfaces has computational complexity of order $O(N)$, where N is the number of cuboids in \mathcal{T} . Iso-surface computation algorithms based on combinatorial approaches have as well a complexity of $O(N)$, but the algorithms do not give the full topological information of the iso-surfaces. More severe, the iso-surface will in general be not complete.

The paper is organized as follows:

In Section 2 we introduce the main definitions and notations. We define the concept of a labeled cuboid graph and its subgraphs. In addition, graph operations on labeled cuboid graphs and on subgraphs are defined. Furthermore, we define iso-paths which are the boundary of iso-elements that will be computed using labeled cuboid graphs. In Section 3, equivalence classes of labeled cuboid graphs and its subgraphs are introduced. Rules for computation of iso-paths of labeled cuboid graphs are given in Section 4. The classification of the different types of labeled cuboid graphs for the computation of iso-paths and iso-path computation rules are given in Section 5. Additionally, the algorithm for a complete iso-path computation of all labeled cuboid graphs \mathcal{T} is given. Furthermore, we include figures illustrating computed iso-surfaces for snap shots of a simulated collision of two liquid droplets and for a crown splash of an impacting droplet. The connectedness of the constructed iso-surface is proven in Section 6. Finally, in Section 7 we give definitions of neighborhoods of iso-paths on which the decomposition of iso-surfaces in connected components is based. Having this decomposition, we show in Section 8 how to efficiently compute iso-surface normals with common orientation on a single component and how to compute a surface region around an iso-point within the component from which discrete mean curvature can be computed.

In this paper we introduce appropriate symbols and definitions which do not always follow the traditional way but efficiently describe the method. Proofs are often given with the help of appropriate figures.

2 Labeled Cuboid Graphs

In this paper a *labeled graph* $G(V, E, \mathcal{F})$ denotes a triple (V, E, \mathcal{F}) of $V \subset \mathbb{R}^3$, $E \subset \mathbb{R}^3$ and $\mathcal{F} : V \rightarrow [0, 1]$ such that V is a set of vertices (nodes), E is a set of edges with end points in V and \mathcal{F} assigns real numbers from $[0, 1]$ as weights (labels) to the nodes.

We call $C \subset \mathbb{R}^3$ a *cuboid* if $C = [a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$. Let $G(V, E, \mathcal{F})$ be a labeled graph. We call $G(V, E, \mathcal{F})$ a *labeled cuboid graph*, if $V = \{P_1, \dots, P_8\}$ and $E = \{e_1, \dots, e_{12}\}$ are the set of vertices and edges of C , respectively. In this case we call C the *cuboid* of G . We say that a graph $H(V_h, E_h, \mathcal{F}_h)$ is a *subgraph* of $G(V, E, \mathcal{F})$ if $V_h \subset V$, $E_h \subset E$, and \mathcal{F}_h is the restriction of \mathcal{F} to V_h .

Let $G(V, E, \mathcal{F})$ be a graph and $P_1, P_2 \in V$. We call P_1 *incident* to P_2 if P_1 and P_2 are the end points of an edge $e \in E$. In case $H(V_h, E_h, \mathcal{F}_h)$ is a subgraph of $G(V, E, \mathcal{F})$ we write " P_1 is incident to P_2 in H " to express the fact that P_1 and P_2 are the end points of an edge $e \in E_h$.

In the present paper, we only consider labeled graphs $G(V, E, \mathcal{F})$ having the following connectivity property: For any node $P_1 \in V$ there exists another node $P_2 \in V$ such that P_1 is incident to P_2 .

Note: If suitable, we use the abbreviation G for a labeled cuboid graph $G(V, E, \mathcal{F})$. Additionally, we sometimes abbreviate a subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G by H and also use the notation $G_i(V_i, E_i, \mathcal{F}_i)$, abbreviated as G_i , for labeled cuboid graphs $G(V_i, E_i, \mathcal{F}_i)$, where $i \in \mathbb{N}$. Analogous abbreviations will be used for subgraphs of G_i . Moreover, we use the shorthand notation G' for the labeled cuboid graph $G(V, E, \mathcal{F}')$; analogously for subgraphs of it.

2.1 Notations

Below we give some notations which will be used in this work. Recall from Notation 1 the symbols $\circ, \ominus, \square, \bullet$ which will be used to indicate the weight of the nodes of a labeled cuboid graph, its subgraphs and iso-points.

Partition of a domain into cuboids: Let $\Omega \subset \mathbb{R}^3$ be a polygonal domain. Here, polygonal domain means a domain with polygonal boundary. We denote by \mathcal{T} the partition of $\overline{\Omega}$ into cuboids such that two cuboids have either a common face or a common vertex or a common edge or they are disjoint. We call such a partition \mathcal{T} of $\overline{\Omega}$ *partition of $\overline{\Omega}$ into cuboids*.

Cuboid grid: Let $\Omega \subset \mathbb{R}^3$ be a polygonal domain and let \mathcal{T} be the partition of $\overline{\Omega}$ into cuboids. Then we call the vertices of all cuboids in \mathcal{T} a cuboid grid.

Parallel faces: We say that two faces F_1 and F_2 of a cuboid C are *parallel*

if both F_1 and F_2 have no common nodes; this is abbreviated by $F_1 \parallel F_2$. In case F_1 and F_2 have common nodes we say that both faces are not parallel, symbolized as $F_1 \nparallel F_2$.

Face subgraph (a face, for short): We say that a graph $H(V_h, E_h, \mathcal{F}_h)$ is a *face subgraph* of a labeled cuboid graph $G(V, E, \mathcal{F})$, if H contains a single face of G and V_h is the set of nodes of the face in H .

Edge subgraph (an edge, for short) or edge: We say that a graph $H(V_h, E_h, \mathcal{F}_h)$ is an *edge subgraph* of a labeled cuboid graph $G(V, E, \mathcal{F})$, if H contains a single edge of G and V_h is the set of nodes of the edge in H .

Face and Edge neighbors: We say that two labeled cuboid graphs $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ are *face-neighbors* if, given C_1 and C_2 as the cuboids of G_1 and G_2 , respectively, the intersection $C_1 \cap C_2$ is a face of both cuboids. We say that two cuboid graphs G_1 and G_2 are *edge-neighbors* if the intersection $C_1 \cap C_2$ is an edge of both cuboids.

2.2 Interpolations and Iso-paths

Suppose we have a labeled cuboid graph $G(V, E, \mathcal{F})$ and an iso-level $c \in (0, 1)$. Then we interpolate linearly between the end points of $e \in E$ and their weights to get a possible point on e with the value c . Then, by connecting two distinct interpolated points of G that lie on the same face of G , we get a line. If, by joining each pair of these points that lie on the same face of G , we obtain a closed path that does not cross itself, we call this path a simple closed path. Any such closed path is the boundary of a continuous 2-dimensional manifold in \mathbb{R}^3 , which will be defined later.

In this section we give notations and definitions which will be used throughout the text.

Definition 2.1. (*Iso-point*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph, $\xi = \cup_{e \in E} e$ the union of all edges of G and $c \in (0, 1)$ be an iso-level. We define a function $f : \xi \rightarrow [0, 1]$ by piecewise definition: on $e \in E$, let f be defined by

$$f(x) = f_0 + (f_1 - f_0) \frac{(x - x_0)}{(x_1 - x_0)} \quad \text{for } x \in e, \quad (1)$$

where x_0 and x_1 are the nodes of e and $f_0 = \mathcal{F}(x_0)$, $f_1 = \mathcal{F}(x_1)$. For $x \in e$ we call the value $f(x)$ the *f-value* of x . If $f(x) = c$ such that $f_0 \leq c < f_1$ or $f_1 \leq c < f_0$ then we call $x \in e$ an *iso-point* of G . For an iso-point $x \in e$ we have

$$x(c) = x_0 + (x_1 - x_0) \frac{c - f_0}{f_1 - f_0}. \quad (2)$$

Iso-nodes, disperse nodes and continuous nodes: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and $c \in (0, 1)$ an iso-level. Then we call all nodes of G with label greater than c *disperse nodes*, otherwise *continuous nodes*. All nodes of G which are iso-points are also called *iso-nodes*. We denote by $D(G)$ the total number of disperse nodes of G .

disperse/continuous graph, face and edge: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and $c \in (0, 1)$ an iso-level. We call G a *disperse graph* if all nodes of G are disperse nodes and in case all nodes of G are continuous we call G a *continuous graph*. A disperse graph G is symbolized as G_{disp} and a continuous graph G is symbolized as G_{cont} . A face subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G is a *disperse face* if all nodes of H are disperse; we call it a *continuous face* if all nodes of H are continuous. We call an edge subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G a *disperse edge* if all nodes of H are disperse; we call it a *continuous edge* if all nodes of H are continuous.

L-face and Trivial L-face: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and $c \in (0, 1)$ an iso-level. We call a face subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G an *L-face* if there exist two disperse and two continuous nodes of H such that the disperse nodes are not incident in H . An L-face $H(V_h, E_h, \mathcal{F}_h)$ is called a *trivial L-face*, if both continuous nodes are iso-nodes. All other L-faces are called *non-trivial L-faces*. We denote by $L(G)$ the set of all L-faces of G . Figure 4 shows all possible L-faces of G .

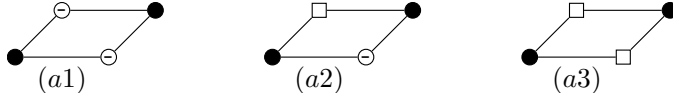


Figure 4: Sketches (a1) and (a2) represent non-trivial L-faces and sketch (a3) represents a trivial L-face.

Singular/regular face: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and $c \in (0, 1)$ an iso-level. A face subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G is called a *singular face* if three nodes of H are disperse and the other node is an iso-node. We say that a face subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G is a *regular face* if H is not an L-face, not a disperse face, not a continuous face and not a singular face. Figure 5 shows all possible regular faces and a singular face in a labeled cuboid graph G .

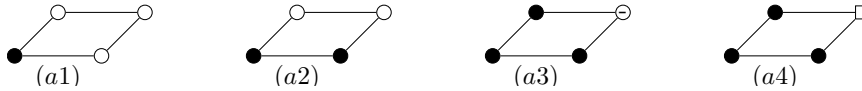


Figure 5: Sketches (a1), (a2) and (a3) represent regular faces and sketch (a4) represents a singular face.

2.2.1 Iso-path and Iso-Elements

The definitions of an iso-element and an iso-path are intertwined to each other. An iso-element is a 2-dimensional manifold in \mathbb{R}^3 composed of flat triangular patches and computed by using the iso-points of a labeled cuboid graph for a given iso-level $c \in (0, 1)$. An iso-path is the boundary of an iso-element.

Cyclically ordered points: Let P_1, \dots, P_n be distinct points in \mathbb{R}^3 , where $n \geq 3$. Suppose that $J = \cup_{i=1}^n e_i$ with $e_i = \overline{P_i P_{i+1}}$ for $i = 1, \dots, n-1$ and $e_n = \overline{P_n P_1}$ is a simply closed path. Then we call the points P_1, \dots, P_n *cyclically ordered* and denote the simply closed path J by $[P_1, \dots, P_n]$.

We denote by $P_c := \frac{1}{n} \sum_{i=1}^n P_i$ the center of $\{P_1, \dots, P_n\}$ and define a surface with boundary $[P_1, \dots, P_n]$ by

$$[P_1, \dots, P_n | P_c] := \cup_{i=1}^{n-1} \text{Tri}(P_c, P_i, P_{i+1}) \cup \text{Tri}(P_c, P_1, P_n), \quad (3)$$

where $\text{Tri}(A, B, C)$ denotes the filled triangle spanned by the points A, B, C of \mathbb{R}^3 . Note that the patches which form such a surface do not lie in a common plane, in general, but for $n = 3$ we have

$$[P_1, P_2, P_3 | P_c] = \text{Tri}(P_1, P_2, P_3).$$

The surface $[P_1, \dots, P_n | P_c]$ is an oriented and connected manifold in \mathbb{R}^3 .

Iso-line: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and $c \in (0, 1)$ be a given iso-level. We say that a line segment l is an *iso-line* of G if its two end points P_1 and P_2 are both iso-points, lying on the same face of the cuboid of G . We then call P_1 incident to P_2 . This defines incidence between iso-points.

Definition 2.2. (*Iso-path and iso-element*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and let $c \in (0, 1)$ be an iso-level. Let G have $n \geq 3$ iso-points Q_1, \dots, Q_n . Let there be a subset $\{P_1, \dots, P_m\} \subset \{Q_1, \dots, Q_n\}$ with $3 \leq m \leq n$ such that the set of line segments $\{P_1 P_2, \dots, P_{m-1} P_m, P_m P_1\}$ is a subset of the set of iso-lines of G . Furthermore, let the iso-points P_1, \dots, P_m define a simply closed path $[P_1, \dots, P_m]$ with P_c being its center. Then we call $[P_1, \dots, P_m]$ an *inner iso-path* of G if $[P_1, \dots, P_m]$ does not lie on a single non-trivial L -face of G .

We call $[P_1, \dots, P_m]$ an *outer iso-path* of G if it lies on a single non-trivial L -face $H(V_h, E_h, \mathcal{F}_h)$ of G and satisfies

$$[P_1, \dots, P_m] = \bigcup_{k \in K} J_k \cap M_h,$$

where $\{J_k\}_{k \in K}$ are the inner iso-paths of G and its face-neighbor $G'(V', E', \mathcal{F}')$, where $V \cap V' = V_h$ and M_h is the common face of the cuboids of G and G' .

We call $[P_1, \dots, P_m]$ an *iso-path* if it is an inner or an outer iso-path, and we then call $[P_1, \dots, P_m | P_c]$ an *iso-element* of G .

Corresponding iso-element, iso-path and iso-line: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and let $c \in (0, 1)$ be an iso-level. Let us denote by ω one of the iso-paths of G and by Z the iso-element which is bounded by all of the edges of ω as given by Definition 2.2. Then we say ω *corresponds to* Z or Z *corresponds to* ω . Furthermore, if l is an iso-line of G which lies in ω then we say that l *corresponds to* ω .

Iso-line neighbor: Let $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ be labeled cuboid graphs and $c \in (0, 1)$ a given iso-level. Assume $G_1 = G_2$ or G_1 and G_2 are face or edge-neighbors according to the given context. Let ω_1 and ω_2 be distinct iso-paths of G_1 and G_2 , respectively. Furthermore, let l_1 and l_2 be iso-lines corresponding to ω_1 and ω_2 , respectively such that l_1 and l_2 have the same end points. Then we call the iso-lines l_1 and l_2 *neighbors*.

Connectedness of iso-path: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph and let $c \in (0, 1)$ be an iso-level. Let ω be an iso-path of G . By definition of an iso-path, ω contains $3 \leq n \leq 6$ iso-lines l_1, \dots, l_n of G . We say that the iso-path ω of G is *connected* if every l_i lies on an iso-path ω_i of G_i , where G_1, \dots, G_n are labeled cuboid graphs with the same iso-level c and $\omega \neq \omega_i$ for all $i = 1, \dots, n$. This means, here *connectedness* refers to *connectedness to all sides of the iso-path*.

Iso-surfaces and connectedness of iso-surfaces: Let $\Omega \subset \mathbb{R}^3$ be a polygonal domain and let \mathcal{T} be the partition of $\bar{\Omega}$ into cuboids. Furthermore, let the vertices of the cuboids in \mathcal{T} be labeled by real weights from $[0, 1]$. Let $c \in (0, 1)$ be an iso-level. Then we call the surfaces obtained by joining all iso-elements of the labeled cuboids in \mathcal{T} *iso-surfaces*. We say that an iso-surface is *connected* if each iso-path which does not have an edge that lies on the boundary of Ω is connected. That means, connected iso-surfaces have *no holes* except, possibly, at the boundary $\partial\Omega$. For further theoretical investigations we here assume that the iso-surfaces do not touch the boundary of Ω .

2.3 Mapping between labeled graphs

Let C be a cuboid with set of vertices V and set of edges E . Then we denote by $\mathbb{G}(V, E)$ the set of all labeled cuboid graphs $G(V, E, \mathcal{F})$ with $\mathcal{F} : V \rightarrow [0, 1]$. Let $q : [0, 1] \rightarrow [0, 1]$ be a given function. Then we define a graph operation $\mathcal{Q} : \mathbb{G} \rightarrow \mathbb{G}$ by

$$G(V, E, \mathcal{F}') = G(V, E, q \circ \mathcal{F}), \quad (4)$$

where $G(V, E, \mathcal{F}) \in \mathbb{G}(V, E)$. We denote by I the identity mapping on $\mathbb{G}(V, E)$.

Definition 2.3. (Subgraph mapping). Let $V_h \subset V$ and $E_h \subset E$, where V and E are the set of vertices and the set of edges of a cuboid C , respectively. Then we denote by $\mathbb{H}(V_h, E_h)$ the set of all subgraphs with set of vertices V_h and set of edges E_h of labeled graphs $G(V, E, \mathcal{F}) \in \mathbb{G}(V, E)$. Let $q_h : [0, 1] \rightarrow [0, 1]$ be a given function. Then we define the graph operation $\mathcal{Q}_h : \mathbb{H}(V_h, E_h) \rightarrow \mathbb{H}(V_h, E_h)$ by

$$\mathcal{Q}_h(H(V_h, E_h, \mathcal{F}_h)) = H(V_h, E_h, \mathcal{F}'_h), \quad (5)$$

where $\mathcal{F}'_h = q_h \circ \mathcal{F}_h$.

Definition 2.4. (Subgraph replacement). Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of the labeled cuboid graph $G(V, E, \mathcal{F})$. Given $q_h : [0, 1] \rightarrow [0, 1]$, we define a function \mathcal{F}' on V by

$$\mathcal{F}' := \begin{cases} \mathcal{F} & \text{on } V \setminus V_h \\ q_h \circ \mathcal{F}_h & \text{on } V_h \end{cases}. \quad (6)$$

We then set

$$G|_{H \rightarrow H'} := G(V, E, \mathcal{F}'), \quad (7)$$

and say that $G|_{H \rightarrow H'}$ is obtained from the graph $G(V, E, \mathcal{F})$ by replacing the subgraph $H(V_h, E_h, \mathcal{F}_h)$ of $G(V, E, \mathcal{F})$ by $H(V_h, E_h, q_h \circ \mathcal{F}_h)$.

Definition 2.5. (Subgraph replacement to a continuous graph). Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of the labeled cuboid graph $G(V, E, \mathcal{F})$. Additionally, let $G'(V, E, \mathcal{F}')$ be a continuous graph with $\mathcal{F}' : V \rightarrow \{0\}$ and let $H'(V_h, E_h, \mathcal{F}'_h)$ be the subgraph of G' corresponding to H . The subgraphs H and H' have the same nodes and edges. Then we define a function $\hat{\mathcal{F}}'$ on V by

$$\hat{\mathcal{F}}' := \begin{cases} \mathcal{F}' & \text{on } V \setminus V_h \\ \mathcal{F}_h & \text{on } V_h \end{cases}. \quad (8)$$

We set

$$G'|_{H' \rightarrow H} := G'(V, E, \hat{\mathcal{F}}'), \quad (9)$$

and say that $G'|_{H' \rightarrow H}$ is obtained from the graph $G'(V, E, \mathcal{F}')$ by replacing the subgraph $H'(V_h, E_h, \mathcal{F}'_h)$ of $G'(V, E, \mathcal{F}')$ by $H(V_h, E_h, \mathcal{F}_h)$.

Definition 2.6. (Subgraph replacement to a disperse graph). Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of the labeled cuboid graph $G(V, E, \mathcal{F})$. Additionally, let $G'(V, E, \mathcal{F}')$ be a disperse graph with $\mathcal{F}' : V \rightarrow \{1\}$ and let $H'(V_h, E_h, \mathcal{F}'_h)$ be the subgraph of G' corresponding to H . The subgraphs H and H' have the same nodes and edges. Then we define a function $\hat{\mathcal{F}}'$ on V by

$$\hat{\mathcal{F}}' := \begin{cases} \mathcal{F}' & \text{on } V \setminus V_h \\ \mathcal{F}_h & \text{on } V_h \end{cases}. \quad (10)$$

We set

$$G'|_{H' \rightarrow H} := G'(V, E, \hat{\mathcal{F}}'), \quad (11)$$

and say that $G'|_{H' \rightarrow H}$ is obtained from the graph $G'(V, E, \mathcal{F}')$ by replacing the subgraph $H'(V_h, E_h, \mathcal{F}'_h)$ of $G'(V, E, \mathcal{F}')$ by $H(V_h, E_h, \mathcal{F}_h)$.

Now we define a so-called general labeled graph $G'(V', E', \mathcal{F}')$ which we get by substituting part of a labeled cuboid graph $G(V, E, \mathcal{F})$ for a given iso-level $c \in (0, 1)$ by a graph, where the nodes of the graph are labeled with values in $[0, 1]$. The graph that will be substituted consists of one or more inner iso-paths of G . Therefore, such a general labeled cuboid graph contains at least one inner iso-path of G .

Definition 2.7. (General labeled graph). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph. Let $V_e \subset \mathbb{R}^3$ be a set of $3 \leq m \leq 4$ points such that each $P \in V_e$ lies on an edge $e \in E$. Let E_e be a given set of edges with end points in V_e . Assume that each $P \in V_e$ is an end point of two edges in the set E_e . Let $\mathcal{F}_e : V_e \rightarrow [0, 1]$ be a labeling on V_e . Then we call $H_e(V_e, E_e, \mathcal{F}_e) := (V_e, E_e, \mathcal{F}_e)$ a labeled graph. Assume that $\mathcal{F}_e = \mathcal{F}$ on $V \cap V_e$. Then we define a labeled graph $\tilde{G}(\tilde{V}, \tilde{E}, \tilde{\mathcal{F}}) := (\tilde{V}, \tilde{E}, \tilde{\mathcal{F}})$ by

$$G(\tilde{V}, \tilde{E}, \tilde{\mathcal{F}}) := (V \cup V_e, E \cup E_e, \tilde{\mathcal{F}}), \quad (12)$$

where

$$\tilde{\mathcal{F}} := \begin{cases} \mathcal{F} & \text{on } V \\ \mathcal{F}_e & \text{on } V_e \end{cases}. \quad (13)$$

Then $\tilde{G}(\tilde{V}, \tilde{E}, \tilde{\mathcal{F}})$ is called a general labeled graph, or labeled graph for short.

Definition 2.8. (General subgraph replacement). Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of the labeled cuboid graph $G(V, E, \mathcal{F})$. Let $\tilde{H}(\tilde{V}, \tilde{E}, \tilde{\mathcal{F}})$ be a labeled graph such that $V_h \subset \tilde{V}$, $E_h \subset \tilde{E}$, $\tilde{V} \subset E_h$ and $\tilde{\mathcal{F}} = \mathcal{F}$ on $V \cap \tilde{V}$. We define a function \mathcal{F}' on $V \cup V_h$ by

$$\mathcal{F}' := \begin{cases} \mathcal{F} & \text{on } V \setminus V_h \\ \mathcal{F}_h & \text{on } V_h \\ \tilde{\mathcal{F}} & \text{on } \tilde{V} \setminus V_h \end{cases}. \quad (14)$$

Then we set

$$G|_{H \rightarrow \tilde{H}} := G(\hat{V}, \hat{E}, \mathcal{F}'), \quad (15)$$

where $\hat{V} = V \cup (\tilde{V} \setminus V_h)$ and $\hat{E} = E \cup (\tilde{E} \setminus E_h)$. We say that $G|_{H \rightarrow \tilde{H}}$ is obtained from the graph $G(V, E, \mathcal{F})$ by replacing the subgraph $H(V_h, E_h, \mathcal{F}_h)$ of $G(V, E, \mathcal{F})$ by the graph $\tilde{H}(\tilde{V}, \tilde{E}, \tilde{\mathcal{F}})$. Note that the labeled graph $G|_{H \rightarrow \tilde{H}}$ may no longer be a labeled cuboid graph.

Note: In this paper, any graph operation applied on a labeled graph with a given iso-level $c \in (0, 1)$ does not change the iso-level c , i.e. the transformed labeled graph has the same iso-level c .

3 Equivalence Classes of Labeled Cuboid Graphs

From here on, whenever we consider (one or several) labeled cuboid graphs, it is understood that also an iso-level $c \in (0, 1)$ has been chosen. We then speak of "a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ ".

For the computation of iso-paths for a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ we compare the node-labels with c . The exact values of the nodes are not important for the investigation of iso-paths of the graph G . Therefore, in the following two definitions we introduce the important concept of equivalence classes of labeled cuboid graphs. The first definition considers for each node of G whether the node is disperse or not. In the second definition of an equivalence class of labeled cuboid graphs, besides the disperse nodes of G , the differences between iso-nodes and nodes with node value less than c are accounted for.

Definition 3.1. Suppose $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ are labeled cuboid graphs with iso-level $c \in (0, 1)$. We call the graphs G_1 and G_2 \circ -equivalent if the following conditions are satisfied:

- (i) $D(G_1) = D(G_2)$,
- (ii) both G_1 and G_2 have the same number of L -faces,
- (iii) to each $Q \in V_1$ with $\mathcal{F}_1(Q) > c$ and $P_1, P_2, P_3 \in V_1$ such that P_1, P_2, P_3 are incident to Q , there exists $Q' \in V_2$ with $\mathcal{F}_2(Q') > c$ and $P'_1, P'_2, P'_3 \in V_2$ such that P'_1, P'_2, P'_3 are incident to Q' and, to each $i = 1, 2, 3$, one of the following holds:
 - (a) if $\mathcal{F}_1(P_i) > c$ then $\mathcal{F}_2(P'_i) > c$,
 - (b) if $\mathcal{F}_1(P_i) \leq c$ then $\mathcal{F}_2(P'_i) \leq c$.

The mapping from Q to Q' is required to be a bijection. We denote the \circ -equivalence between G_1 and G_2 by $G_1 \iff_{\circ} G_2$. Additionally, we denote by $[G_1(V_1, E_1, \mathcal{F}_1)]_{\circ}$ the \circ -equivalence class, defined by

$$[G_1(V_1, E_1, \mathcal{F}_1)]_{\circ} := \{G(V, E, \mathcal{F}) : G \iff_{\circ} G_1\}. \quad (16)$$

Definition 3.2. Suppose $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ are labeled cuboid graphs with iso-level $c \in (0, 1)$. We call the graphs G_1 and G_2 \square -equivalent if the following conditions are satisfied:

- (i) $D(G_1) = D(G_2)$,
- (ii) both G_1 and G_2 have the same number of L -faces,

(iii) to each $Q \in V_1$ with $\mathcal{F}_1(Q) > c$ and $P_1, P_2, P_3 \in V_1$ such that P_1, P_2, P_3 are incident to Q , there exists $Q' \in V_2$ with $\mathcal{F}_2(Q') > c$ and $P'_1, P'_2, P'_3 \in V_2$ such that P'_1, P'_2, P'_3 are incident to Q' and, to each $i = 1, 2, 3$, one of the following holds:

- (a) if $\mathcal{F}_1(P_i) > c$ then $\mathcal{F}_2(P'_i) > c$,
- (b) if $\mathcal{F}_1(P_i) < c$ then $\mathcal{F}_2(P'_i) < c$,
- (c) if $\mathcal{F}_1(P_i) = c$ then $\mathcal{F}_2(P'_i) = c$.

The mapping from Q to Q' is required to be a bijection. We denote the \square -equivalence between G_1 and G_2 by $G_1 \iff_{\square} G_2$. Additionally, we denote by $[G_1(V_1, E_1, \mathcal{F}_1)]_{\square}$ the \square -equivalence class, defined by

$$[G_1(V_1, E_1, \mathcal{F}_1)]_{\square} := \{G(V, E, \mathcal{F}) : G \iff_{\square} G_1\}. \quad (17)$$

Illustration of \circ -equivalence class: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $V = \{P_1, \dots, P_8\}$ be the nodes of G and let C be the cuboid of G . Consider a sketch that shows the edges and vertices of C , and such that the vertices of C are marked as follows:

- (i) P_i is marked by \bullet if $\mathcal{F}(P_i) > c$,
- (ii) P_i is marked by \circ if $\mathcal{F}(P_i) \leq c$.

Then we say that the sketch represents $[G(V, E, \mathcal{F})]_{\circ}$.

Illustration of \square -equivalence class: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $V = \{Q_1, \dots, Q_m, P_{m+1}, \dots, P_8\}$ with $m = D(G)$ be the nodes of G , where $\mathcal{F}(Q_i) > c$ for $i = 1, \dots, m$ and $\mathcal{F}(P_j) \leq c$ for $j = m+1, \dots, 8$. Let C be the cuboid of G . Consider a sketch that shows the edges and vertices of C , and such that the vertices of C are marked as follows:

- (i) Q_i is marked by \bullet for all $i \in \{1, \dots, m\}$,
- (ii) P_i is marked by \circ for all $i \in \{m+1, \dots, 8\}$ with $\mathcal{F}(P_i) \leq c$ and P_i is not incident to any one of the nodes in $\{Q_1, \dots, Q_m\}$,
- (iii) P_i is marked by \ominus for all $i \in \{m+1, \dots, 8\}$ with $\mathcal{F}(P_i) < c$ and P_i is incident to one of the nodes in $\{Q_1, \dots, Q_m\}$,
- (iv) P_i is marked by \square for all $i \in \{m+1, \dots, 8\}$ with $\mathcal{F}(P_i) = c$ and P_i is incident to any one of the nodes in $\{Q_1, \dots, Q_m\}$.

Then we say that the sketch represents $[G(V, E, \mathcal{F})]_{\square}$.

Sketches will be "numbered" by (a), (b), (c), ... or, (a1), (a2), ... throughout this paper. Examples for \circ - and \square -equivalence classes are given in Figure 6.

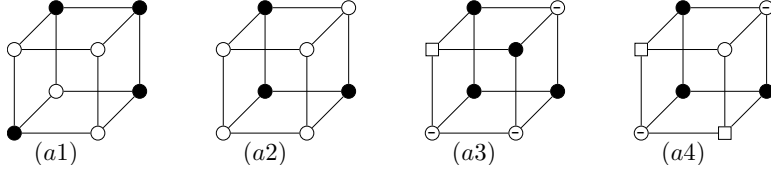


Figure 6: Sketches $(a1), \dots, (a4)$ represent equivalence classes $[(a1)]_\circ$, $[(a2)]_\circ$, $[(a3)]_\square$ and $[(a4)]_\square$, respectively.

Equivalence class of a subgraph: Suppose $H(V_h, E_h, \mathcal{F}_h)$ is a subgraph of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. Then we denote by $[H(V_h, E_h, \mathcal{F}_h)]_\circ$ the \circ -equivalence class of H such that each element in $[H(V_h, E_h, \mathcal{F}_h)]_\circ$ satisfies Definition 3.1 restricted to $H(V_h, E_h, \mathcal{F}_h)$. Analogously, we denote by $[H(V_h, E_h, \mathcal{F}_h)]_\square$ the \square -equivalence class of H such that each element in $[H(V_h, E_h, \mathcal{F}_h)]_\square$ satisfies Definition 3.2 restricted to $H(V_h, E_h, \mathcal{F}_h)$.

Illustration of \circ - and \square -equivalence subclasses: Analogously to \circ - and \square -equivalence classes, we can represent both subclasses by sketches. Given a sketch (a) , we denote by $[(a)]_\circ$ and $[(a)]_\square$ the equivalence classes of the graph or subgraph represented by (a) .

Figure 7 illustrates some examples of \circ - and \square -equivalence subclasses.



Figure 7: Sketches $(b1), \dots, (b4)$ are representations of equivalence subclasses $[(b1)]_\circ$, $[(b2)]_\circ$, $[(b3)]_\square$ and $[(b4)]_\square$, respectively.

Finally, we define an additional class of labeled cuboid graphs which we call $\circ-\star$ -class and $\square-\star$ -class, where for certain nodes no restriction on the label is done.

Definition 3.3. Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $\tilde{V} \subset V$. Then we define the $\circ-\star$ -class of G corresponding to \tilde{V} by

$$[G(V, E, \mathcal{F}; \tilde{V})]_\circ^* := \bigcup_{\tilde{\mathcal{F}} \in \mathbb{F}} [G(V, E, \tilde{\mathcal{F}})]_\circ, \quad (18)$$

where

$$\mathbb{F} = \{\hat{\mathcal{F}} : V \longrightarrow [0, 1] \mid \hat{\mathcal{F}} = \mathcal{F} \text{ on } V \setminus \tilde{V}\}. \quad (19)$$

Definition 3.4. Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $\tilde{V} \subset V$. Then we define the $\square-\star$ -class of G corresponding to \tilde{V} by

$$[G(V, E, \mathcal{F}; \tilde{V})]_{\square}^{\star} := \bigcup_{\tilde{\mathcal{F}} \in \mathbb{F}} [G(V, E, \tilde{\mathcal{F}})]_{\square}, \quad (20)$$

where

$$\mathbb{F} = \{\hat{\mathcal{F}} : V \longrightarrow [0, 1] \mid \hat{\mathcal{F}} = \mathcal{F} \text{ on } V \setminus \tilde{V}\}. \quad (21)$$

Illustration of $\circ-\star$ -class: Suppose a sketch (a) represents $[G(V, E, \mathcal{F})]_{\circ}$, i.e. $[(a)]_{\circ} = [G(V, E, \mathcal{F})]_{\circ}$. Consider a sketch (\tilde{a}) which is a copy of (a) but those nodes in \tilde{a} corresponding to $\tilde{V} \subset V$ are marked by the symbol \diamond . We then say that (\tilde{a}) represents $[G(V, E, \mathcal{F}; \tilde{V})]_{\circ}^{\star}$ and write $[(\tilde{a})]_{\circ}^{\star}$ for this.

Illustration of $\square-\star$ -equivalence class: Suppose a sketch (a) represents $[G(V, E, \mathcal{F})]_{\square}$, i.e. $[(a)]_{\square} = [G(V, E, \mathcal{F})]_{\square}$. Consider a sketch (\tilde{a}) which is a copy of (a) but those nodes in \tilde{a} corresponding to $\tilde{V} \subset V$ are marked by the symbol \diamond . We then say that (\tilde{a}) represents $[G(V, E, \mathcal{F}; \tilde{V})]_{\square}^{\star}$ and write $[(\tilde{a})]_{\square}^{\star}$ for this.

$\circ-\star$ -subclass and $\square-\star$ -subclass: Suppose $H(V_h, E_h, \mathcal{F}_h)$ is a subgraph of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. Let $\tilde{V} \subset V$ and assume $\tilde{V}_h = V_h \cap \tilde{V} \neq \emptyset$. With an analogous definition as (18) for $H(V_h, E_h, \mathcal{F}_h)$, we get the $\circ-\star$ -subclass of $H(V_h, E_h, \mathcal{F}_h)$ corresponding to \tilde{V}_h which is denoted by $[H(V_h, E_h, \mathcal{F}_h; \tilde{V}_h)]_{\circ}^{\star}$. With an analogous definition as (20) for $H(V_h, E_h, \mathcal{F}_h)$, we get the $\square-\star$ -subclass of $H(V_h, E_h, \mathcal{F}_h)$ corresponding to \tilde{V}_h which is denoted by $[H(V_h, E_h, \mathcal{F}_h; \tilde{V}_h)]_{\square}^{\star}$.

Illustration of $\circ-\star$ -subclass and $\square-\star$ -subclass: Suppose $[(a)]_{\circ} = [H(V_h, E_h, \mathcal{F}_h)]_{\circ}$, i.e. the sketch (a) represents $[H(V_h, E_h, \mathcal{F}_h)]_{\circ}$. Consider a sketch (\tilde{a}) which is a copy of (a) but the nodes in \tilde{a} corresponding to $\tilde{V}_h \subset V_h$ are marked by the symbol \diamond . We then say that (\tilde{a}) represents $[H(V_h, E_h, \mathcal{F}_h; \tilde{V}_h)]_{\circ}^{\star}$ and write $[(\tilde{a})]_{\circ}^{\star}$ for this. If we start with $[(a)]_{\square} = [H(V_h, E_h, \mathcal{F}_h)]_{\square}$ instead, we obtain a sketch \tilde{a} that represents the subclass $[H(V_h, E_h, \mathcal{F}_h; \tilde{V}_h)]_{\square}^{\star}$; we write $[(\tilde{a})]_{\square}^{\star}$ for this.

Figure 8 shows examples of $\circ-\star$ - and $\square-\star$ -classes and subclasses with iso-level $c \in (0, 1)$.

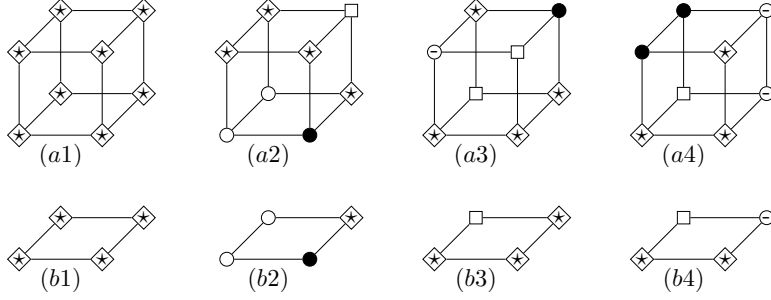


Figure 8: Sketches (a1) and (a2) represent $\circ-\star$ -classes and sketches (a3) and (a4) represent $\square-\star$ -classes. Sketches (b1) and (b2) represent $\circ-\star$ -subclasses and sketches (b3) and (b4) represent $\square-\star$ -subclasses.

Notation 2. Sometimes we use sketches which can have either all four symbols $\circ, \ominus, \square, \bullet$ or all three symbols \circ, \ominus, \bullet to represent a class of labeled cuboid graphs or subgraphs of it. These special sketches that we use in the next sections are given in Figure 9. We call the equivalence classes represented by the sketches (a1), (a2) and (a3) the \square -equivalence classes and the equivalence class represented by the sketch (a4) the \square -equivalence subclass.

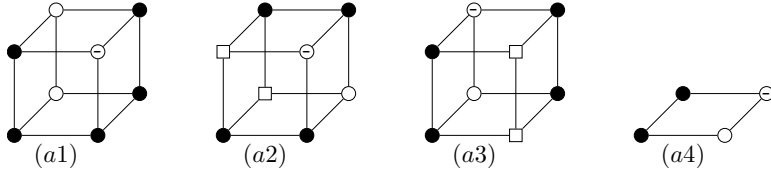


Figure 9: Sketches (a1), (a2) and (a3) represent \square -equivalence classes and sketch (a4) represents \square -equivalence subclass.

4 Rules of Iso-path Computations

In this section we define mappings that will be applied on $\mathbb{G}(V, E)$. They will be used for the computation of iso-paths in labeled cuboid graphs with iso-level $c \in (0, 1)$. These mappings replace subgraphs of a graph by other graphs just as described by Definitions 2.4 and 2.8.

The distinction between different types of face subgraphs of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ introduced in Section 2 is important for the computation of iso-paths of G . We illustrate by Figure 10 the different types of faces of G . Sketch (a1) represents the $\circ-\star$ -subclass $[(a1)]_{\circ}^{\star}$ of regular faces and sketch (a2) represents the \square -equivalence subclass $[(a2)]_{\square}$ of regular faces. Sketch (a3) represents the \square -equivalence subclass of singular faces. Sketches (a4), (a5) and (a6) represent the possible \circ - and \square -

equivalence subclasses of L-faces. Here $[(a5)]_{\square}$ is a \square -equivalence subclass of trivial L-faces and $[(a6)]_{\square}$ is a \square -equivalence subclass of non-trivial L-faces.

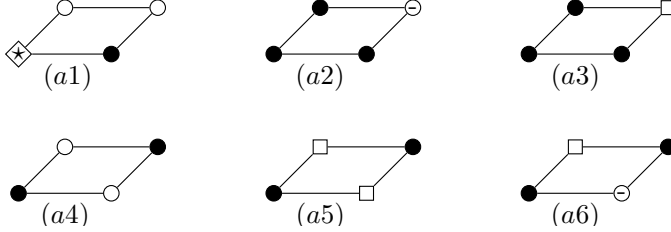


Figure 10: Sketches (a1), ..., (a6) illustrate the different types of face sub-graphs.

4.1 Removing Singular and Isolated Iso-paths

Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. In this section we introduce graph operations on G which are called T -rules and F -rules. The T -rules are denoted by T_1 and T_2 and remove *singular iso-paths* in G , where a singular iso-path is a degenerate closed path with only one or two nodes. Singular iso-paths correspond to iso-elements of surface measure zero. The T_1 -rule removes singular iso-paths with only one node and the T_2 -rule removes singular iso-paths with two nodes.

The F -rules are graph operations denoted by F_1 and F_2 . The F_1 -rule removes iso-paths in G such that the iso-element computed from the iso-paths separates only disperse nodes of G . The F_2 -rule removes an iso-path of G if G has the labeled cuboid graph $G'(V', E', \mathcal{F}')$ with the same iso-level c as a face neighbor and both G and G' contain four iso-nodes and four disperse nodes such that the iso-nodes lie on the common face. In this case, the iso-element computed from the iso-path separates only the disperse nodes of both face neighboring graphs. An iso-path of G which is removed using the F_1 - or F_2 -rule is called an *isolated iso-path*.

Isolated iso-element: An iso-element computed from an isolated iso-path is called an *isolated iso-element*.

Regular labeled cuboid graph: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is neither a disperse nor a continuous graph. Furthermore, assume G has neither singular iso-paths nor an isolated iso-path. Then we call G a *regular labeled cuboid graph*. Sometimes we use the abbreviation G is *regular* instead of G is a regular labeled cuboid graph.

4.1.1 T- and F-graphs

In this section we introduce the T-subgraphs and F-graphs of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. The existence of such graphs in G is a possible indication of singular iso-path or isolated iso-path existence in G . The detection of isolated iso-paths is necessary for the computation of iso-paths of G , since isolated iso-paths may not be connected. Removing isolated iso-paths guarantees the iso-path connectedness as will be shown in Section 6.

Definition 4.1. (*T₁-subgraph*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of G such that the following conditions hold:

1. the number of points in V_h is four ($|V_h| = 4$),
2. there exist a point $P' \in V_h$ such that P' is incident to all points $P \in V_h \setminus \{P'\}$ in H and

$$\mathcal{F}_h(P') = c \quad \text{and} \quad \mathcal{F}_h(P) > c \quad \forall P \in V_h \setminus \{P'\}.$$

Then H is called a T_1 -subgraph.

Definition 4.2. (*T₂-subgraph*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of G such that the following conditions hold:

1. the number of points in V_h is seven ($|V_h| = 7$),
2. there exist two points $P_1, P_2 \in V_h$ such that P_1 is incident to P_2 in H and

$$\mathcal{F}_h(P_1) = \mathcal{F}_h(P_2) = c \quad \text{and} \quad \mathcal{F}_h(P) > c \quad \forall P \in V_h \setminus \{P_1, P_2\}.$$

Then H is called a T_2 -subgraph.

T_1 - and T_2 -subgraphs are subsumed as T -subgraphs.

Definition 4.3. (*F₁-graph*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let there be $\tilde{V} \subset V$ with $|\tilde{V}| = 4$ and

1. each $P \in \tilde{V}$ is incident only to two points in $V \setminus \tilde{V}$,
2. $\mathcal{F}(P) = c \quad \forall P \in \tilde{V}$,
3. $\mathcal{F}(P) > c \quad \forall P \in V \setminus \tilde{V}$.

Then G is called an F_1 -graph.

Definition 4.4. (F_2 -graph). Suppose $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ are face-neighbored labeled cuboid graphs with iso-level $c \in (0, 1)$. Let the following properties hold:

1. $\mathcal{F}_1(P) = \mathcal{F}_2(P) = c \quad \forall P \in V_1 \cap V_2$,
2. $\mathcal{F}_1(P) > c \quad \forall P \in V_1 \setminus (V_1 \cap V_2)$,
3. $\mathcal{F}_2(P) > c \quad \forall P \in V_2 \setminus (V_1 \cap V_2)$.

Then G_1 is called an F_2 -graph.

F_1 - and F_2 -graphs are subsumed as F -graphs.

Figure 11 illustrates the T -subgraphs and F -graphs. The sketches (a) and (b) shown in Figure 11 represent the equivalence subclasses $[(a)]_\square$ and $[(b)]_\square$. The T_1 - and T_2 -subgraphs lie in $[(a)]_\square$ and $[(b)]_\square$, respectively. The sketches (c), (d₁), (d₂) in Figure 11 represent $[(c)]_\square$, $[(d_1)]_\square$ and $[(d_2)]_\square$, respectively. The F_1 -graph lies in $[(c)]_\square$ and the F_2 -graph lies in $[(d_1)]_\square$ as well as in $[(d_2)]_\square$.

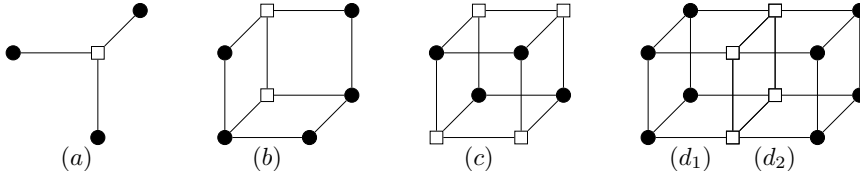


Figure 11: Sketches (a) and (b) represent T_1 - and T_2 -subgraphs, respectively and F_1 - and F_2 -graphs are represented by sketch (c) and the sketches (d₁), (d₂), respectively.

4.1.2 T- and F-rules

A labeled cuboid graph $G(V, E, \mathcal{F}) \in \mathbb{G}(V, E)$ with iso-level $c \in (0, 1)$ can have one to four singular iso-paths or an isolated iso-path, but not both types of iso-paths. This section is devoted to the indication and deletion of singular iso-paths or of an isolated iso-path.

Let $G(V, E, \mathcal{F}) \in \mathbb{G}(V, E)$ and $c \in (0, 1)$ be an iso-level. Let $q_0, q_1 : [0, 1] \rightarrow [0, 1]$ be defined by

$$q_0(x) := \begin{cases} 0 & \text{if } x > c \\ x & \text{else} \end{cases} \quad (22)$$

and

$$q_1(x) := \begin{cases} 1 & \text{if } x \leq c \\ x & \text{else} \end{cases} . \quad (23)$$

Let $W \subset V$. We define mappings $Q_0, Q_1 : \mathbb{G}(V, E) \longrightarrow \mathbb{G}(V, E)$ by $Q_0(G(V, E, \mathcal{F})) = G(V, E, \mathcal{R}_0)$ and $Q_1(G(V, E, \mathcal{F})) = G(V, E, \mathcal{R}_1)$, where

$$\mathcal{R}_0 := \begin{cases} \mathcal{F} & \text{on } V \setminus W \\ q_0 \circ \mathcal{F} & \text{on } W \end{cases} \quad (24)$$

and

$$\mathcal{R}_1 := \begin{cases} \mathcal{F} & \text{on } V \setminus W \\ q_1 \circ \mathcal{F} & \text{on } W \end{cases}. \quad (25)$$

Definition 4.5. (T_1 -rule). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a T_1 -subgraph of G . We call the mapping Q_1 , defined by setting $W := V_h$ in (25), a T_1 -rule. If required for clarity, we speak of the T_1 -rule with respect to H .

Definition 4.6. (T_2 -rule). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a T_2 -subgraph of G . We call the mapping Q_1 , defined by setting $W := V_h$ in (25), a T_2 -rule. If required for clarity, we speak of the T_2 -rule with respect to H .

We subsume the T_1 - and T_2 -rules as T -rules.

Definition 4.7. (T_1^* -rule). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let G have $1 \leq n \leq 4$ distinct T_1 -subgraphs, denoted as $H_1(V_{h_1}, E_{h_1}, \mathcal{F}_{h_1}), \dots, H_n(V_{h_n}, E_{h_n}, \mathcal{F}_{h_n})$. We consider four cases, where in the case $i \in \{1, \dots, n\}$, the T_1 -rule changes the node values of H_i according to:

1. Case $i = 1$: $G_1(V, E, \mathcal{F}_1) := T_1(G(V, E, \mathcal{F}))$ (T_1 -rule w.r. to H_1)
2. Case $i = 2$: $G_2(V, E, \mathcal{F}_2) := T_1(G_1(V, E, \mathcal{F}_1))$ (T_1 -rule w.r. to H_2)
3. Case $i = 3$: $G_3(V, E, \mathcal{F}_3) := T_1(G_2(V, E, \mathcal{F}_2))$ (T_1 -rule w.r. to H_3)
4. Case $i = 4$: $G_4(V, E, \mathcal{F}_4) := T_1(G_3(V, E, \mathcal{F}_3))$ (T_1 -rule w.r. to H_4).

Then we write

$$T_1^*(G(V, E, \mathcal{F})) := G_n(V, E, \mathcal{F}_n). \quad (26)$$

We call this T_1^* -rule. If we apply the T_1^* -rule to G then $T_1^*(G)$ will have no more T_1 -subgraphs.

Definition 4.8. (F -rules). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let G be an F_1 - or an F_2 -graph. Let $V_h = \{P_1, P_2, P_3, P_4\} \subset V$ be such that $\mathcal{F}(P) = c$ for all $P \in V_h$. Then we call the mapping Q_1 , defined by setting $W := V_h$ in (25), an F_1 -rule or an F_2 -rule if G is an F_1 - or F_2 -graph, respectively. The F_1 - and F_2 -rules are denoted by F_1 and F_2 , respectively.

We subsume the F_1 - and F_2 -rules as F -rules.

The T - and F -rules are illustrated in Figure 12 and 13, respectively. The sequence 1 and 2 in Figure 12 represents T_1 - and T_2 -rules, respectively. The sequence 1 and 2 in Figure 13 represents F_1 - and F_2 -rules, respectively.

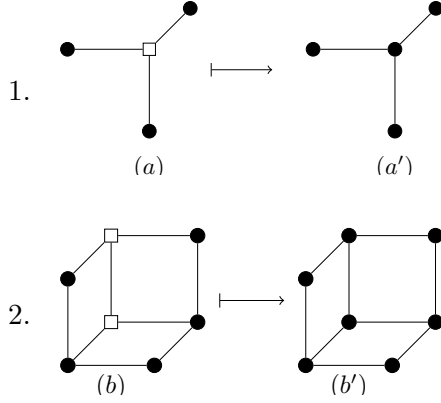


Figure 12: The sequence 1 and 2 illustrate the T_1 - and T_2 -rules, respectively.

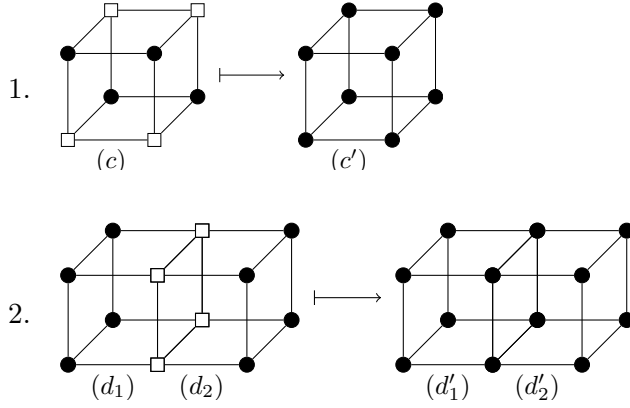


Figure 13: The sequence 1 and 2 illustrate the F_1 - and F_2 -rules, respectively.

The following result about singular faces will be proved using T -rules.

Proposition 4.9. (*Singular faces*). *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let G be regular. Suppose that G has a singular face. Then the maximum number of singular faces which G can have is three. Furthermore, if G has $n = 2$ or $n = 3$ singular faces then there exist a total of n iso-points which are iso-nodes in G such that these iso-nodes lie on the singular faces. Then each pair of these iso-nodes lies on a regular face of G or on a space diagonal of the cuboid of G . Moreover, an iso-node can never be on two distinct singular faces.*

Proof. We give the proof of Proposition 4.9 by using Figure 14. If $G \in [(a1)]_{\square}^*$ then G has at least one singular face. The other possibilities for G to have two singular faces occur only if $G \in [(a2)]_{\square}$ or $G \in [(a3)]_{\circ}$. The only possibility for G to have three singular faces is $G \in [(a4)]_{\square}$. The singular faces are marked by bold lines as displayed in Figure 14. There is no possibility to get more than three singular faces of G . The pair of iso-nodes

corresponding to singular faces of G in case (a2) and (a4) lies on regular face diagonals of G . But in case (a3) the pair of iso-nodes corresponding to singular faces of G lies on a diagonal of the cuboid of G . Furthermore, the rule T_1 forbids the possibility of an iso-node being on two distinct singular faces, which proves the last claim. \square

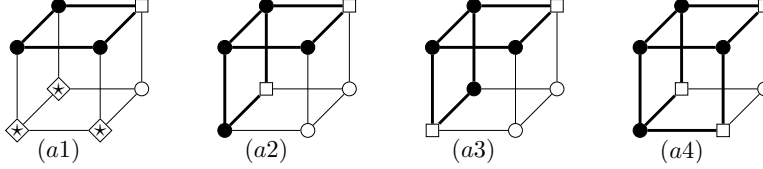


Figure 14: Sketches (a1), (a2), (a3) and (a4) illustrate the possibilities of a labeled cuboid graph to have singular faces.

4.2 Iso-path Computation Rules

In this section we give rules for iso-path computation for a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. We consider two types of rules which are called S -rules and C -rules. S -rules compute iso-paths in G , whereas C -rules compute iso-lines in G . By combining C - and S -rules we get the iso-paths in G . Furthermore, consecutive application of C -rules to a labeled cuboid graph G , on which no S -rules apply gives an additional iso-path in G .

In this section we consider not only labeled cuboid graphs but as well iso-points, iso-lines and iso-paths. We also give graphical sketches to illustrate for a given labeled cuboid graph the corresponding iso-points, iso-lines and iso-paths. Figure 15 illustrates that for $G(V, E, \mathcal{F}) \in [(a1)]_{\square}$ the iso-points on the edges are marked by the symbol \square as shown in sketch (a2), and the iso-lines that connect two iso-points on a face are marked by $\square-\square$ as shown in sketch (a3). The simple closed path shown in sketch (a3) is an iso-path of G .

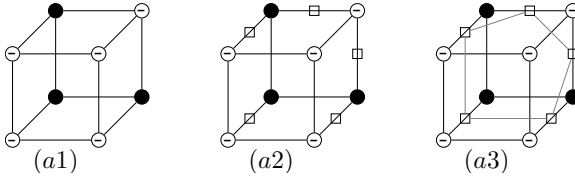


Figure 15: Sketches (a1), (a2) and (a3) illustrate the steps of iso-path computation.

4.2.1 S -subgraphs, S -cuboid graphs and S -rules

Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. The S -rules are denoted by S_1, S_2, S_3 and will be applied on $G(V, E, \mathcal{F})$ for computing and deleting iso-paths of G . They are graph operations which will be applied on so-called S -subgraphs of G as described below.

Definition 4.10. (S_1 -subgraph). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of G such that the following conditions hold:

1. the number of points in V_h is four ($|V_h| = 4$),
2. there exist a point $P' \in V_h$ such that P' is incident to all points $P \in V_h \setminus \{P'\}$ in H and

$$\mathcal{F}_h(P') > c \quad \text{and} \quad \mathcal{F}_h(P) \leq c \quad \forall P \in V_h \setminus \{P'\}.$$

Then H is called an S_1 -subgraph.

Definition 4.11. (S_2 -subgraph). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of G such that the following conditions hold:

1. the number of points in V_h is six ($|V_h| = 6$),
2. there exist two points $P_1, P_2 \in V_h$ such that P_1 is incident to P_2 in H , each P_1 and P_2 are incident in H to three points in V_h and

$$\mathcal{F}_h(P_1) > c, \quad \mathcal{F}_h(P_2) > c \quad \text{and} \quad \mathcal{F}_h(P) \leq c \quad \forall P \in V_h \setminus \{P_1, P_2\}.$$

Then H is called an S_2 -subgraph.

Definition 4.12. (S_3 -subgraph). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a subgraph of G such that the following conditions hold:

1. the number of points in V_h is four ($|V_h| = 4$),
2. there exist a point $P' \in V_h$ such that P' is incident to all points $P \in V_h \setminus \{P'\}$ in H and

$$\mathcal{F}_h(P') < c \quad \text{and} \quad \mathcal{F}_h(P) > c \quad \forall P \in V_h \setminus \{P'\}.$$

Then H is called an S_3 -subgraph.

S_1 -, S_2 - and S_3 -subgraphs are subsumed as S -subgraphs.

In Figure 16, sketches (a), (b) and (c) represent $[(a)]_\circ$, $[(b)]_\circ$ and $[(c)]_\square$, respectively. The S_1 -, S_2 - and S_3 -subgraphs are elements of $[(a)]_\circ$, $[(b)]_\circ$ and $[(c)]_\square$, respectively.

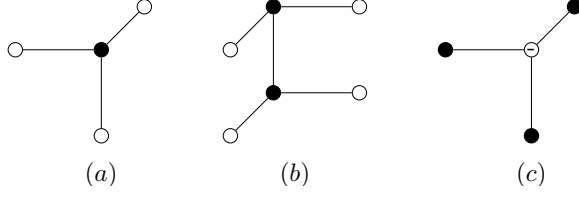


Figure 16: The sketches (a), (b) and (c) illustrate S_1 -, S_2 - and S_3 -subgraphs, respectively.

Definition 4.13. (*S-cuboid graphs*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be an S_1 -subgraph of G . Then by using Definition 2.5 we get a labeled cuboid graph $G'|_{H' \rightarrow H}$, where H' and G' are defined as given by the Definition 2.5. Then we call $G'|_{H' \rightarrow H}$ the S_1 -cuboid graph corresponding to H . If H is an S_2 -subgraph of G then we call $G'|_{H' \rightarrow H}$ the S_2 -cuboid graph corresponding to H . Analogously, in case H is an S_3 -subgraph of G using Definition 2.6 we get a labeled cuboid graph $G'|_{H' \rightarrow H}$, where H' and G' are defined as given by the Definition 2.6. Then we call $G'|_{H' \rightarrow H}$ the S_3 -cuboid graph corresponding to H .

S_1 -, S_2 - and S_3 -cuboid graphs are subsumed as S -cuboid graphs.

In Figure 17, sketches (a), (b) and (c) represent $[(a)]_\circ$, $[(b)]_\circ$ and $[(c)]_\square$, respectively. The S_1 -, S_2 - and S_3 -cuboid graphs are elements of $[(a)]_\circ$, $[(b)]_\circ$ and $[(c)]_\square$, respectively.

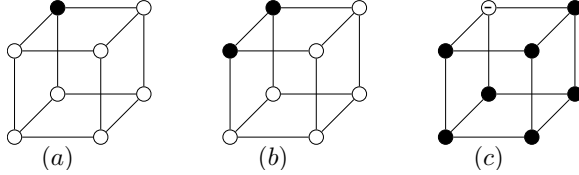


Figure 17: The sketches (a), (b) and (c) illustrate S_1 -, S_2 - and S_3 -cuboid graphs, respectively.

Definition 4.14. (*Subgraph with iso-path*). Let $H(V_h, E_h, \mathcal{F}_h)$ be an S_1 - or S_3 -subgraph and let $c \in (0, 1)$ be an iso-level. Let $V_{iso} = \{P \in e : e \in E_h, P \text{ an iso-point}\}$ be the set of iso-points corresponding to H . Let $E_{iso} = \{e = \overline{P_i P_j} : P_i, P_j \in V_{iso} \text{ and } P_i \neq P_j\}$. Then we define a labeled graph $\tilde{H}(\tilde{V}_h, \tilde{E}_h, \tilde{\mathcal{F}}_h)$, where $\tilde{V}_h = V_h \cup V_{iso}$, $\tilde{E}_h = E_h \cup E_{iso}$ and

$$\tilde{\mathcal{F}}_h = \begin{cases} \mathcal{F}_h & \text{on } V_h, \\ c & \text{on } V_{iso}. \end{cases} \quad (27)$$

We call \tilde{H} an S_1 - or S_3 -subgraph with iso-path if H is an S_1 - or S_3 -subgraph, respectively.

Definition 4.15. (*Subgraph with iso-path*). Let $H(V_h, E_h, \mathcal{F}_h)$ be an S_2 -subgraph and let $c \in (0, 1)$ be an iso-level. Let $V_{iso} = \{P \in e : e \in E_h, P \text{ an iso-point}\}$ be the set of iso-points corresponding to H . Let $E_{iso} = \{e = \overline{P_i P_j} : P_i, P_j \in V_{iso} \text{ with } P_i \neq P_j \text{ and } P_1, \dots, P_4 \text{ are cyclically ordered}\}$. Then we define a labeled graph $\tilde{H}(\tilde{V}_h, \tilde{E}_h, \tilde{\mathcal{F}}_h)$, where $\tilde{V}_h = V_h \cup V_{iso}$, $\tilde{E}_h = E_h \cup E_{iso}$ and

$$\tilde{\mathcal{F}}_h = \begin{cases} \mathcal{F}_h & \text{on } V_h, \\ c & \text{on } V_{iso}. \end{cases} \quad (28)$$

We call \tilde{H} an S_2 -subgraph with iso-path.

S_1 -, S_2 - and S_3 -subgraphs with iso-path are subsumed as S -subgraphs with iso-path. In Figure 18, sketches (a'), (b') and (c') represent S_1 -, S_2 - and S_3 -subgraphs with iso-paths, respectively.

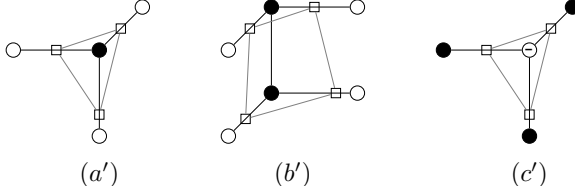


Figure 18: Sketches (a'), (b') and (c') illustrate S_1 -, S_2 - and S_3 -subgraphs with iso-paths, respectively.

In the following three definitions we use the functions q_0 and q_1 defined by (22) and (23).

Definition 4.16. (*Iso-path free subgraph*). Let $H(V_h, E_h, \mathcal{F}_h)$ be an S_i -subgraph ($i = 1, 2, 3$) and let $c \in (0, 1)$ be an iso-level. Then we call the labeled graph $H(V_h, E_h, \mathcal{R}_h)$ an iso-path free S_i -subgraph, where $\mathcal{R}_h = q_0 \circ \mathcal{F}_h$ in case $i = 1, 2$ and $\mathcal{R}_h = q_1 \circ \mathcal{F}_h$ if $i = 3$. Iso-path free S_1 -, S_2 - and S_3 -subgraphs are subsumed as iso-path free S -subgraphs.

In Figure 19, sketches (a''), (b'') and (c'') illustrate the iso-path free S_1 -, S_2 - and S_3 -subgraphs which are contained in $[(a'')]_{\circ}$, $[(b'')]_{\circ}$ and $[(c'')]_{\circ}$, respectively.

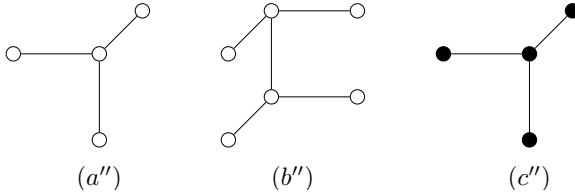


Figure 19: Sketches (a''), (b'') and (c'') illustrate iso-path free S_1 -, S_2 - and S_3 -subgraphs, respectively.

Let $H(V_h, E_h, \mathcal{F}_h)$ be an S -subgraph of $G(V, E, \mathcal{F})$ and let $c \in (0, 1)$ be an iso-level. Then there exists an iso-path of G , since we have a corresponding S -subgraph with iso-path. This iso-path is as well an iso-path of G . In the overall iso-surface construction, the iso-paths that we get from S -graphs will be recorded in a list. Thereafter, the S -subgraph is substituted in G with an iso-path free S -subgraph. Hence we get from G a new labeled cuboid graph $G'(E, V, \mathcal{F}')$ with a new labeling and a reduced number of iso-paths. The complete procedure of computing an iso-path of G corresponding to an S -subgraph, recording the corresponding iso-path and then substituting the S -subgraph in G with an iso-path free subgraph is called an S -rule. These S -rules are also called S_1 -, S_2 - and S_3 -rules if they correspond to the S_1 -, S_2 - and S_3 -subgraphs, respectively.

The symbols used in the following two definitions have been introduced in Definition 2.8.

Definition 4.17. (*S -rule on a labeled cuboid graph*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let $H(V_h, E_h, \mathcal{F}_h)$ be an S_1 -subgraph of G . Let $\tilde{H}(\tilde{V}_h, \tilde{E}_h, \tilde{\mathcal{F}}_h)$ be the S_1 -subgraph with iso-path corresponding to H . In addition, let $\hat{H}(V_h, E_h, q_0 \circ \mathcal{F}_h)$ be the iso-path free S_1 -subgraph corresponding to H . Then we call the following sequence an S_1 -rule of G corresponding to H :

$$G \longrightarrow G|_{H \rightarrow \tilde{H}} \longrightarrow G|_{H \rightarrow \hat{H}}. \quad (29)$$

Likewise, we define for S_2 - and S_3 -subgraphs the corresponding S_2 - and S_3 -rules on G , using the labelings $q_0 \circ \mathcal{F}_h$ and $q_1 \circ \mathcal{F}_h$, respectively. We subsume the S_1 -, S_2 - and S_3 -rules on G as S -rules.

Definition 4.18. (*S^n -rules on a labeled cuboid graph*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let $H_1(V_{h_1}, E_{h_1}, \mathcal{F}_{h_1})$, $H_2(V_{h_2}, E_{h_2}, \mathcal{F}_{h_2})$ be S_1 -subgraphs of G . Let $\tilde{H}_1(\tilde{V}_{h_1}, \tilde{E}_{h_1}, \tilde{\mathcal{F}}_{h_1})$ and $\tilde{H}_2(\tilde{V}_{h_2}, \tilde{E}_{h_2}, \tilde{\mathcal{F}}_{h_2})$ be S_1 -subgraphs with iso-paths corresponding to H_1 and H_2 , respectively. In addition, let $\hat{H}_1(V_{h_1}, E_{h_1}, q_0 \circ \mathcal{F}_{h_1})$ and $\hat{H}_2(V_{h_2}, E_{h_2}, q_0 \circ \mathcal{F}_{h_2})$ be the iso-path free S_1 -subgraphs corresponding to H_1 and H_2 , respectively. Then we call the following sequence an S_1^2 -rule of G , corresponding to H_1 and H_2 :

$$\begin{aligned} G &\longrightarrow G|_{H_1 \rightarrow \tilde{H}_1} \longrightarrow G|_{H_1 \rightarrow \hat{H}_1} =: G'(V, E, \mathcal{F}') \\ G' &\longrightarrow G'|_{H_2 \rightarrow \tilde{H}_2} \longrightarrow G'|_{H_2 \rightarrow \hat{H}_2}. \end{aligned}$$

Likewise, we define for S_2 - and S_3 -subgraphs the S_2^2 - and S_3^2 -rules of G . In analogy, we define S_1^3 -rules. All these S -rules will be subsumed as S^n -rules, where $n \in \{1, 2, 3\}$ if the type of S -rule is S_1 or $n \in \{1, 2\}$ if the type of S -rule is S_2 or S_3 .

The S -rules will be written in a simplified *graph-theoretical rules* as displayed in Figure 20.

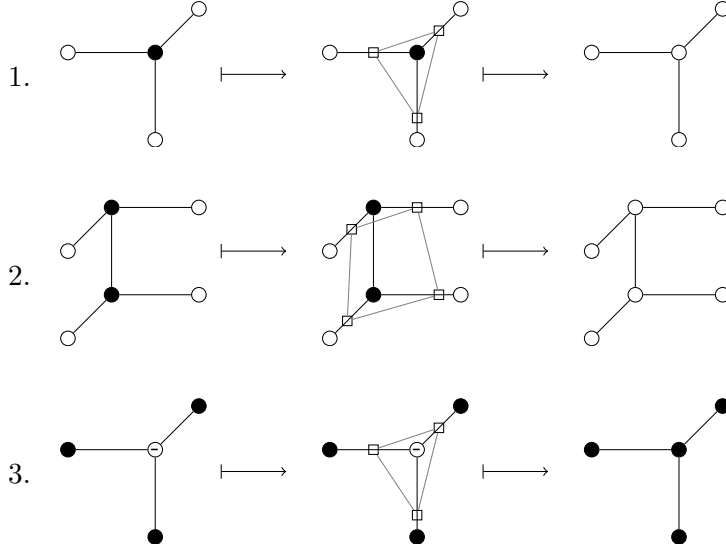


Figure 20: The sequence 1, 2 and 3 represent the S_1 -, S_2 - and S_3 -rules, respectively.

4.2.2 C -subgraphs and C -rules

In this section we describe the so-called C -rules. C -rules are graph operations which operate on the regular faces of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. Applying a C -rule to a regular face of G gives an iso-line that lies on this face.

Definition 4.19. (C -subgraphs). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $H(V_h, E_h, \mathcal{F}_h)$ be a regular face subgraph of G such that one of the following properties is satisfied:

1. H contains one disperse node,
2. H contains two disperse nodes,
3. H contains three disperse nodes.

In case H satisfies 1 we call H a C_1 -subgraph. Likewise, we call H a C_2 - or a C_3 -subgraph if H satisfies 2 or 3, respectively. We subsume the C_1 -, C_2 - and C_3 -subgraphs as C -subgraphs. C -subgraphs are regular faces and vice versa.

Definition 4.20. (C -subgraphs with iso-lines and C -rules). Let $H(V_h, E_h, \mathcal{F}_h)$ be a C_1 -subgraph and let $c \in (0, 1)$ be an iso-level. Let $V_{iso} = \{P \in e : e \in E_h \text{ and } P \text{ is iso-point}\}$ be the set of iso-points corresponding to H . Let $E_{iso} = \{e = \overline{P_i P_j} : P_i, P_j \in V_{iso} \text{ and } P_i \neq P_j\}$. Then we define a labeled

graph $\tilde{H}(\tilde{V}_h, \tilde{E}_h, \tilde{\mathcal{F}}_h)$, where $\tilde{V}_h = V_h \cup V_{iso}$, $\tilde{E}_h = E_h \cup E_{iso}$ and

$$\tilde{\mathcal{F}}_h = \begin{cases} \mathcal{F}_h & \text{on } V_h, \\ c & \text{on } V_{iso}. \end{cases} \quad (30)$$

We call \tilde{H} a C_1 -subgraph with iso-line. Analogously, we define C_2 - and C_3 -subgraphs with iso-lines in case H is a C_2 -subgraph or a C_3 -subgraph, respectively. We subsume these subgraphs as C -subgraphs with iso-lines. In addition, we call the transformation process which takes H to a C_k -subgraph with iso-line a C_k -rule ($k = 1, 2, 3$). The C_1 -, C_2 - and C_3 -rules are subsumed as C -rules.

The C -rules will be written in a simplified *graph-theoretical rules* as shown in Figure 21.

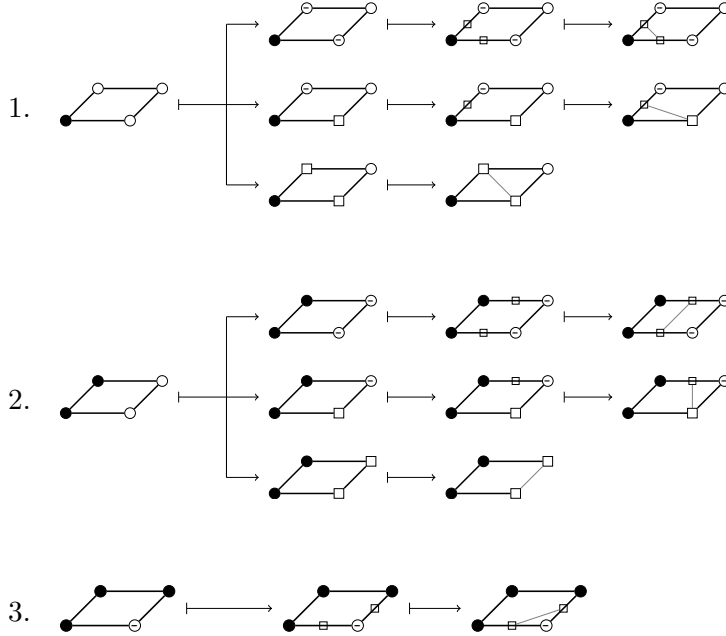


Figure 21: The sequence 1, 2 and 3 illustrate the C_1 -, C_2 - and C_3 -rules, respectively.

Note: A singular face contains only one iso-point and hence it is not possible to compute an iso-line on it. Therefore, C -rules will not be applied to singular faces.

Proposition 4.21. *The application of any of the C -rules as well as any of the S -rules to a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ gives the same iso-lines on the regular faces of G .*

Proof. Both C - and S -rules compute iso-lines by connecting iso-points on the same face of $G(V, E, \mathcal{F})$. Since a regular face of G has only two iso-points

we only get one iso-line on the face. Therefore, the C - and S -rules give the same iso-line on a regular face G . \square

Notation 3. (Corresponding node or nodes of iso-line and corresponding iso-path). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be regular. Let $H(V_h, E_h, \mathcal{F}_h)$ be a regular face of G , having one or two or three disperse nodes (cf. sketches (a1), (a2) and (a3) of Figure 22). Note that in case H has three disperse nodes then the fourth (continuous) node of H is not allowed to be an iso-node, since otherwise H is a singular face. Let l be the iso-line of H which is computed by applying either the C_1 -, or C_2 - or the C_3 -rule to H . The types of the C -rules which will be applied to H are chosen according to the graph-theoretical rules as given in Figure 21. Then we say that the disperse node or nodes of H correspond to the iso-line l .

Now, let $H'(V'_h, E'_h, \mathcal{F}'_h)$ be a non-trivial L-face of G (cf. sketches (a4) and (a5) of Figure 22). Let P be one of the continuous nodes of H' and let P be not an iso-node. Note that at least one continuous node of a non-trivial L-face is not an iso-node, since otherwise H is a trivial L-face. By joining the iso-points in H' that are incident to P in H' , we get an iso-line l and we say that the continuous node P corresponds to the iso-line l . Moreover, if there exists an inner iso-path ω of G that passes through l we say that ω corresponds to P . Additionally, let Q be one of the disperse nodes of H' . By joining the iso-points in H' that are incident to Q in H' , we get an iso-line l and we say that the disperse node Q corresponds to the iso-line l . Furthermore, if there exists an inner iso-path ω of G that passes through l we say that ω corresponds to Q .

The sketches (a1), (a2) and (a3) in Figure 22 show cases with an iso-line on a regular face. In case (a1) the iso-line on the face corresponds to the disperse node of the face and in the other two cases each of the iso-lines on the faces corresponds to the disperse nodes of the face. The Sketches (a4) and (a5) in Figure 22 show non-trivial L-faces with possible iso-lines. Iso-lines corresponding to the continuous node (denoted by \ominus) are drawn bold for (a4) and (a5), while iso-lines corresponding to disperse nodes are drawn light.

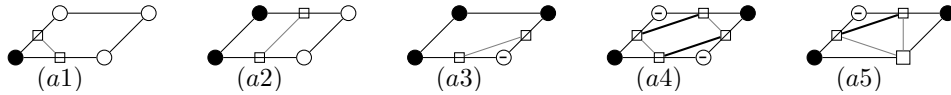


Figure 22: Sketches (a1), (a2) and (a3) show cases with an iso-line on a regular face. Sketches (a4) and (a5) show cases with iso-lines on non-trivial L-faces.

5 Classification of Labeled Cuboid Graphs and Computation of Iso-paths

The primary objective of this section is to find a correspondence between iso-paths and subgraphs of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. The secondary objective of this section is to find the set of subgraphs of G that correspond to the complete set of iso-paths of G , without knowing the iso-paths of G . Finally, we give an algorithm to find the set of subgraphs of G that correspond to the complete set of *inner iso-paths* of G , where an *inner iso-path* is an iso-path of G which does not lie on a single non-trivial L-face of G .

For these purposes we define three different types of labeled subgraphs of G as follows:

1. subgraphs of surface measure zero which do not lie on a face of the cuboid of G ,
2. subgraphs of positive surface measure which do not lie on a face of the cuboid of G ,
3. L-face subgraphs, lying on a face of the cuboid of G .

Subgraphs of G of surface measure zero which do not lie on a face of the cuboid of G correspond to an iso-element without surface area. The possible surface measure zero subgraphs of G are illustrated by the sketches (a) and (b) in Figure 23. We denote by \hat{g}_1 and \hat{g}_2 arbitrary subgraphs contained in the \square -equivalence classes $[(a)]_\square$ and $[(b)]_\square$, respectively. The subgraphs \hat{g}_1 and \hat{g}_2 are denoted *basic zero subgraphs* of a labeled cuboid graph, since any surface measure zero subgraph of G contains \hat{g}_1 or \hat{g}_2 as a subgraph.

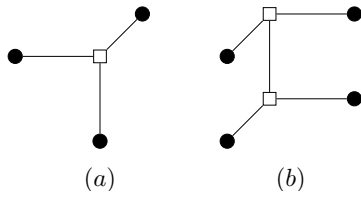


Figure 23: Sketches (a) and (b) illustrate basic zero subgraphs of a labeled cuboid graph. The labeled subgraphs corresponding to (a) and (b) are denoted by \hat{g}_1 and \hat{g}_2 , respectively.

Subgraphs of G of positive surface measure which do not lie on a face of the cuboid of G correspond to iso-elements with positive surface area. If we change the disperse nodes of \hat{g}_1 and \hat{g}_2 to continuous nodes and the iso-node of \hat{g}_1 and the iso-nodes of \hat{g}_2 to disperse nodes then we get labeled graphs denoted by g_1 and g_2 , respectively. The labeled graphs g_1 and g_2 are

contained in the \circ -equivalence classes $[(a)]_\circ$ and $[(b)]_\circ$, respectively, where sketches (a) and (b) are shown in Figure 24. If we change the iso-node of graph \hat{g}_1 to a label less than the iso-value c then we get a labeled graph denoted by g_3 which is contained in the \square -equivalence class $[(c)]_\square$, where sketch (c) is given in Figure 24.

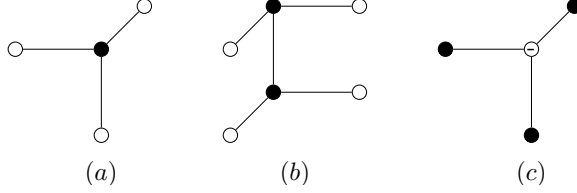


Figure 24: The sketches (a), (b) and (c) illustrate basic positive subgraphs of a labeled cuboid graph. The labeled subgraphs corresponding to (a), (b) and (c) are denoted by g_1 , g_2 and g_3 , respectively.

The labeled graphs g_1 , g_2 and g_3 have positive surface measure and are called *basic positive subgraphs* of a labeled cuboid graph. Here "basic positive subgraphs" means that the surface measure that we get from the labeled graphs g_1 , g_2 and g_3 is positive and they have the smallest number of edges compared to other positive surface measure subgraphs which do not lie on a face of a labeled cuboid graph.

Now we give a definition which characterizes the positive surface measure subgraphs of a labeled cuboid graph which contain a single iso-path of the graph which does not lie on a single non-trivial L-face of the graph.

Definition 5.1. (*Reduced positive surface measure subgraph*). Let $G(V, E, \mathcal{F})$ be a regular labeled cuboid graph with iso-level $c \in (0, 1)$. Then we call the subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G a *reduced positive surface measure subgraph* if either H is in $[g_1]_\circ$, or if H has at least two disperse nodes and satisfies the following conditions:

1. H contains all incidence relations present in G between the disperse nodes of G ,
2. for any two different disperse nodes of H there exists a path which connects both disperse nodes such that the path passes only through disperse edges of H ,
3. all continuous nodes of G which are incident to the disperse nodes of H are in H and these are the only continuous nodes in H ,
4. any edge $e \in E_h$ has at least one disperse node as an end point,
5. H contains no L-faces,
6. H does not contain two different subgraphs of G which are in $[g_3]_\square$.

The labeled graphs contained in the \circ -equivalence classes $[(a1)]_\circ, \dots, [(a4)]_\circ$, where sketches $(a1), \dots, (a4)$ are given in Figure 25, illustrate examples of reduced positive surface measure subgraphs which are not basic positive subgraphs.

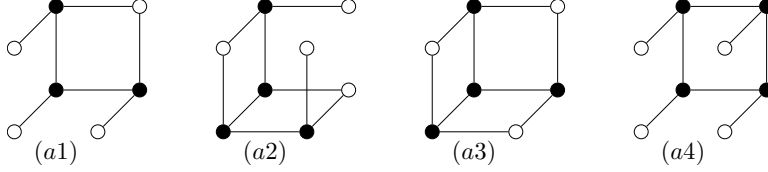


Figure 25: Sketches $(a1)$ to $(a4)$ illustrate reduced positive surface measure subgraphs of a labeled cuboid graph which are not basic and do not lie on a face.

The existence of basic positive measure subgraphs in a labeled cuboid graph G with iso-level $c \in (0, 1)$ induces a classification of G as reducible or irreducible as will be defined in the next subsection.

5.1 Classification of a Labeled Cuboid Graph

Let $G(V, E, \mathcal{F})$ be a regular labeled cuboid graph with iso-level $c \in (0, 1)$. Then G can be reducible or irreducible. This classification of regular graphs is important for the computation of iso-paths. Reducible labeled cuboid graphs will be transformed stepwise to irreducible labeled cuboid graphs, using the S -rules. Each step of transformation from reducibility to irreducibility of a labeled cuboid graph G gives an iso-element of G and, furthermore, an irreducible labeled cuboid graph has a single iso-element.

Any regular labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ has precisely one of the following properties

- (a) G is L-face free,
- (b) G has only non-trivial L-faces,
- (c) G has one trivial L-face.

If G is regular and L-face free then it has one of the following forms:

1. there exist two disperse nodes such that each of them is incident only to continuous nodes,
2. there exist two continuous nodes such that each of them is incident only to disperse nodes,
3. all nodes satisfy none of the conditions given by 1 and 2 from above.

Recall that $L(G)$ is the set of all L-faces of a labeled cuboid graph G with iso-level $c \in (0, 1)$ and $D(G)$ denotes the number of disperse nodes of G .

Definition 5.2. (*Reducible/irreducible labeled cuboid graph*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be regular. Then we call G reducible if one of the following conditions holds:

1. $L(G) \neq \emptyset$,
2. $D(G) = 2$ and there is $H(V_h, E_h, \mathcal{F}_h) \in [g_1]_\circ$ such that $H \subset G$,
3. $D(G) = 6$ and there is $H(V_h, E_h, \mathcal{F}_h) \in [g_3]_\square$ such that $H \subset G$.

We call G irreducible if G is not reducible.

Note: Reducible and irreducible labeled cuboid graphs are regular. A reducible labeled cuboid graph contains at least two inner iso-paths, while an irreducible labeled cuboid graph has one iso-path.

Reducible graphs will be decomposed with respect to inner iso-paths using the basic positive subgraphs. Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is reducible. Then there are $n \in \{1, 2, 3\}$ and $i \in \{1, 2, 3\}$ such that S_i^n -rule is applicable on G and

$$\text{the set of inner iso-paths of } G \text{ is } L_1 \cup L_2, \quad (31)$$

where L_1 is the set of all inner iso-paths that we get by applying the S_i^n -rule to G and L_2 is the iso-path of a *reduced positive surface measure subgraph* $H'(V'_h, E'_h, \mathcal{F}'_h)$ of a labeled cuboid graph $G'(V', E', \mathcal{F}')$ (with the same iso-level c), where G' and G have the same set of nodes and H' contains all disperse nodes of G' . We call G' a *rest graph* of G . This means there exists a decomposition χ of G with respect to inner iso-paths of G as

$$\chi(G) = (S_{i,1}, \dots, S_{i,n}, R), \quad (32)$$

where $S_{i,1}, \dots, S_{i,n}$ denote the n distinct S_i -subgraphs of G and R is the rest graph of G which we get after we apply the S_i^n -rule to G . The rest graph R of G is irreducible. In addition, we define a decomposition η of G into labeled cuboid graphs (with the same iso-level c) by

$$\eta(G) := (G_1, \dots, G_n, R), \quad (33)$$

where G_l is the l -th S_i -cuboid graph of G for $l = 1, \dots, n$ and R is the rest graph of G . Note that the G_l are irreducible labeled cuboid graphs. By the definition of the l -th S_i -cuboid graph of G , the following holds:

- for all $l = 1, \dots, n$, the iso-path of G_l is the same as the iso-path that we get by applying the S_i^l -rule to G .

Theoretical investigations and algorithmical computation of iso-surfaces and surface normals corresponding inner iso-paths of G are easier if we use the labeled cuboid graphs G_l for $l = 1, \dots, n$ and the rest graph R of G as given by the decomposition (33) instead of G .

5.2 Inner Iso-paths of Labeled Cuboid Graphs

In this section we compute inner iso-paths of a given labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$. For the computation of the inner iso-paths we repeatedly refer to the labeled graphs g_1 , g_2 and g_3 as explained above in this section.

Theorem 5.3. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is regular and has at least one L -face. Then G contains a subgraph $H(V_h, E_h, \mathcal{F}_h)$ which is an element of $[g_1]_\circ$ or $[g_2]_\circ$ or $[g_3]_\square$.*

Proof. We consider each case from $D(G) = 2$ to $D(G) = 6$, separately. In the following, G is an element of a \circ - or \square -equivalence class represented by the sketch of a labeled cuboid graph as shown on the left side of the figures below. We use as well special cases of \square -equivalence for G as given in Notation 2.

1. $D(G) = 2$: see Figure 26. Evidently, there is $H \in [g_1]_\circ$.

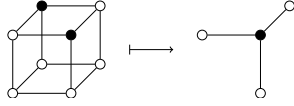


Figure 26: The left part represents $[G]_\circ$ such that $D(G) = 2$ and $L(G) \neq \emptyset$.

2. $D(G) = 3$: see Figure 27. In case of sketch (a) we have $H \in [g_1]_\circ$ and in case of sketch (b) we have $H \in [g_1]_\circ$ and $H \in [g_2]_\circ$.

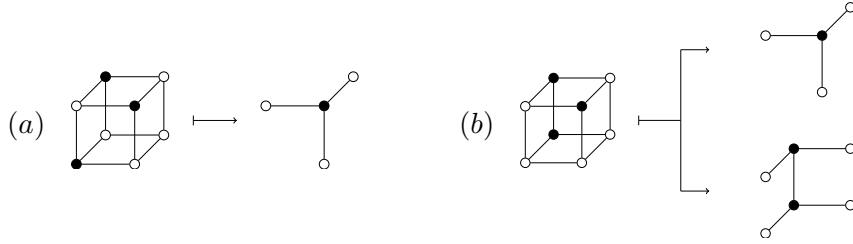


Figure 27: The left side of the sketches (a) and (b) represent the two possibilities of G such that $D(G) = 3$ and $L(G) \neq \emptyset$.

3. $D(G) = 4$: see Figure 28. In case of sketch (a) we have $H \in [g_1]_\circ$ and in case of sketch (b) we have $H \in [g_2]_\circ$.

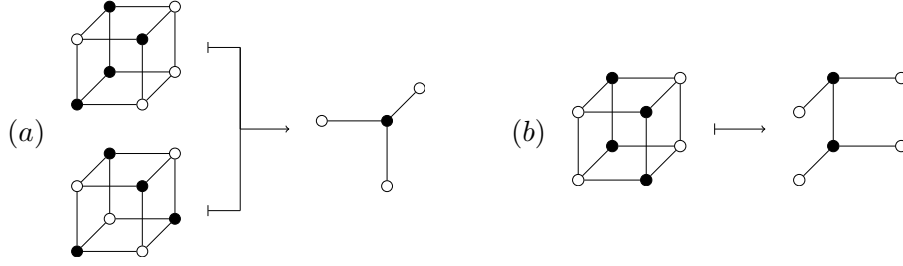


Figure 28: The left side of the sketches (a) and (b) represent the three possibilities of G such that $D(G) = 4$ and $L(G) \neq \emptyset$.

4. $D(G) = 5$: see Figure 29. In case of sketch (a) we have $H \in [g_1]_\circ$ and $H \in [g_3]_\square$ and in case of sketch (b) we have $H \in [g_3]_\square$.

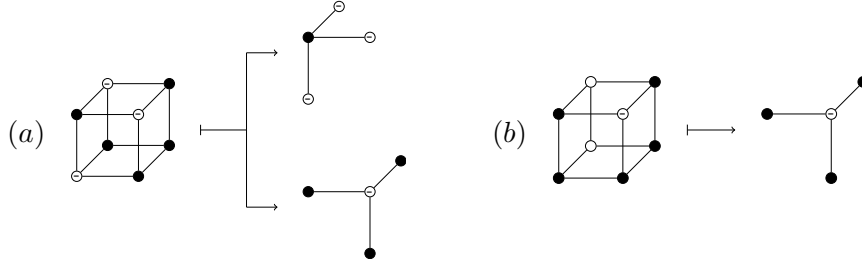


Figure 29: The left side of the sketches (a) and (b) represent the two possibilities of G such that $D(G) = 5$ and $L(G) \neq \emptyset$.

5. $D(G) = 6$: see Figure 30. It holds that $H \in [g_3]_\square$.

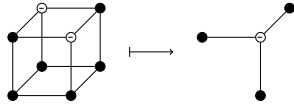


Figure 30: The sketch on the left represents $[G]_\square$ such that $D(G) = 6$ and $L(G) \neq \emptyset$. □

Note: A labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ and $D(G) = 1$ or $D(G) = 7$ has no L-faces, since on any L-face there exists two disperse and two continuous nodes.

Propositions 5.4 and 5.5 draw consequences of Theorem 5.3.

Proposition 5.4. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be regular. Then, if G has L-faces at all, the numbers of possible L-faces in dependence of $D(G)$ is given in Table 1 .*

Proposition 5.5. (*Removing L-faces*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Suppose that G is regular and has at least one L-face. If an S^n -rule is chosen according to row three of Table 1 and if we apply this S^n -rule to G , we get an L-face free labeled cuboid graph $G(V, E, \mathcal{F}')$. Here, $n \in \{1, 2, 3\}$ has to be chosen according to row three of Table 1. The computation of \mathcal{F}' is described in Definition 4.18. Here we denote by $|L(G)|$ the total number of L-faces in G and, as before, $D(G)$ denotes the number of disperse nodes of G .

$D(G)$	2		3		4			5		6
$ L(G) $	1	1	3	2			6	1	3	1
S^n -rule	S_1	S_1	S_1^2	L-faces \nparallel S_1	L-faces \parallel S_2	S_1^3	S_3	S_1	S_3	
S -rule	S_1	S_1		S_1	S_2	S_1	S_3	S_1	S_3	

Table 1: Rules for removing L-faces. The signs \parallel and \nparallel correspond to parallel and non-parallelity of the L-faces in case of two L-faces.

We get the results of Proposition 5.4 and 5.5 given in Table 1 by the same arguments as used to prove Theorem 5.3 for the cases $D(G) = 2$ to $D(G) = 6$. Therefore, a detailed proof is omitted.

Note: From here on, when we say that an S -rule applies on a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$, where G has at least one L-face, it is understood that the corresponding S -rule is chosen according to Table 1. Moreover, if we say that we apply the S_i -rule ($i \in \{1, 2, 3\}$) to G , it is understood that the S_i -rule is chosen according to Table 1.

Proposition 5.6. Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is regular with at least one L-face and $2 \leq D(G) \leq 6$. Suppose the subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G is an L-face. Let the S -rule that will be applied on G be chosen according to Table 1. If the S_1 - or S_2 -rule is applied on G then one of the two disperse nodes of H is the disperse node of an S_1 - or S_2 -subgraph of G , respectively. If the S_3 -rule is applied on G then one of the two continuous nodes of H which is not an iso-node is the continuous node of an S_3 -subgraph of G .

Proof. Choosing the S -rule for G according to Table 1 and using the arguments used to prove Theorem 5.3 proofs the claim. \square

Theorem 5.7. Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is regular and $D(G) \in \{2, 6\}$. Suppose that G has no L-face and let one of the following hold:

- (a) for $D(G) = 2$, the two disperse nodes are on the diagonal of the cuboid of G ,
- (b) for $D(G) = 6$, the two continuous nodes are on the diagonal of the cuboid of G .

Then G contains two subgraphs $H(V_h, E_h, \mathcal{F}_h)$ and $H'(V'_h, E'_h, \mathcal{F}'_h)$ which are in $[g_1]_\circ$ for the case (a) and in $[g_3]_\square$ for the case (b), respectively.

Proof. In the following, G is an element of the \circ -equivalence class represented by the sketch of a labeled cuboid graph as shown on the left side of the figures below.

1. Case $D(G) = 2$: see Figure 31. Evidently, there is $H, H' \in [g_1]_\circ$.

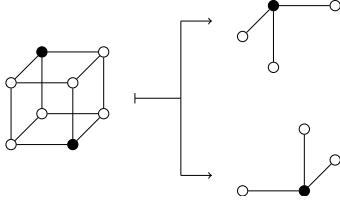


Figure 31: The sketch on the left represents $[G]_\circ$ such that $D(G) = 2$ and the two disperse nodes are on the space diagonal of the cuboid of G .

2. Case $D(G) = 6$: see Figure 32. Evidently, there is $H, H' \in [g_3]_\square$.

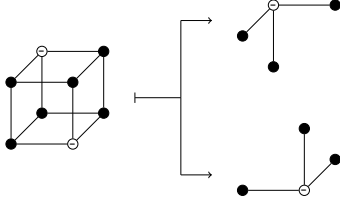


Figure 32: The sketch on the left represents $[G]_\square$ such that $D(G) = 6$ and the two continuous nodes are on the space diagonal of the cuboid of G . \square

Proposition 5.8. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be irreducible. Then the following holds:*

1. $1 \leq D(G) \leq 7$,
2. G has no L -face,
3. if $D(G) = 2$ or $D(G) = 6$ then G satisfies neither the assumption (a) nor (b) of Theorem 5.7.

Proof. The results follow using Table 1 and Theorem 5.7 and the fact that G is as well irreducible in case $D(G) = 1$ or $D(G) = 7$. \square

Theorem 5.9. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G contain only one reduced positive surface measure subgraph $H(V_h, E_h, \mathcal{F}_h)$ and let H contain all disperse nodes of G . Then G is irreducible and hence contains only one iso-path. Vice versa, if G is irreducible then there exists a subgraph of G which satisfies the above stated properties of H .*

Proof. We give the prove by computing the iso-paths of G by joining the iso-points with iso-lines. The steps of the iso-path computation are given in each case by figures with a sequence of sketches from left to right. The symbols on the rightmost side with only disperse or only continuous nodes are used to characterize the resulting type of inner iso-path. The sketch on the left shows the respective labeled cuboid graph, in the second sketch the iso-points are marked and in the third sketch the iso-lines are inserted by applying the C -rules. The sketch on the right shows the resulting iso-path.

1. $D(G) \neq 2$ and $D(G) \neq 6$.

(a) $D(G) = 1$: see Figure 33.

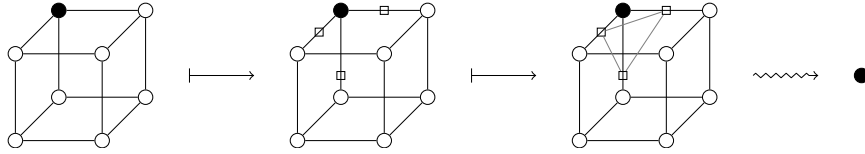


Figure 33: Computation of the iso-path if $D(G) = 1$.

(b) $D(G) = 3$: see Figure 34.

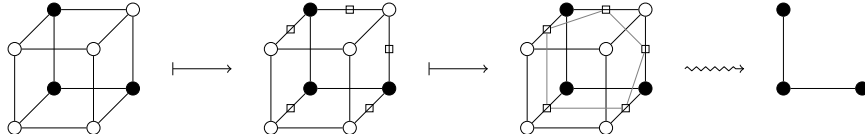


Figure 34: Computation of the iso-path if $D(G) = 3$ and $L(G) = \emptyset$.

(c) $D(G) = 4$: see Figure 35.

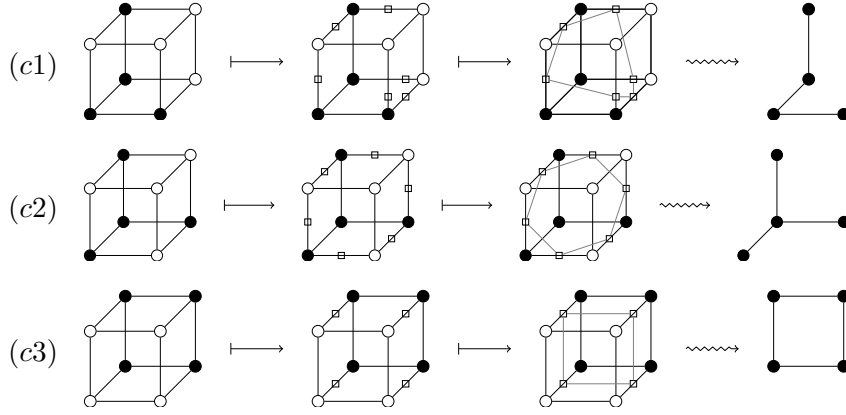


Figure 35: Computation of the iso-path if $D(G) = 4$ and $L(G) = \emptyset$ in three different cases as shown by the sketches (c1), (c2) and (c3).

(d) $D(G) = 5$: see Figure 36.

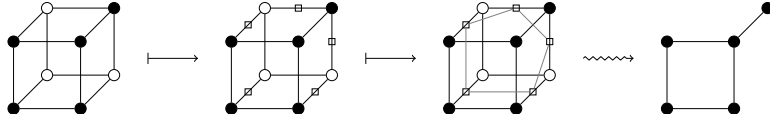


Figure 36: Computation of the iso-path if $D(G) = 5$ and $L(G) = \emptyset$.

(e) $D(G) = 7$: see Figure 37.

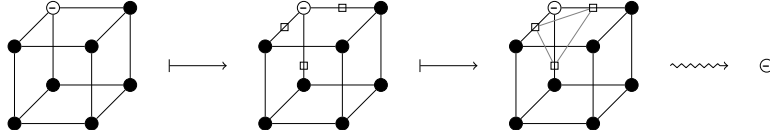


Figure 37: Computation of the iso-path if $D(G) = 7$.

2. $D(G) = 2$ or $D(G) = 6$.

(a) $D(G) = 2$: see Figure 38.

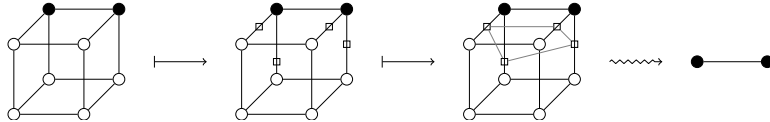


Figure 38: Computation of the iso-path if $D(G) = 2$ and both disperse nodes lie on the same edge of the cuboid of G .

(b) $D(G) = 6$: see Figure 39.

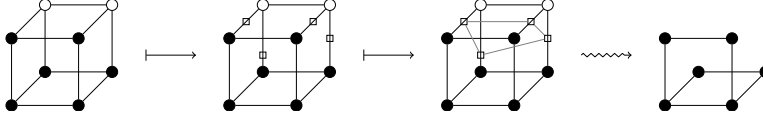


Figure 39: Computation of the iso-path if $D(G) = 6$ and the two continuous nodes lie on the same edge of the cuboid of G .

The simple paths constructed above are iso-paths, since they satisfy the criteria for an inner iso-path given in Definition 2.2. Furthermore, in all cases, G contains only one reduced positive surface measure subgraph containing all disperse nodes of G . Therefore, G is irreducible.

To show the last statement, observe that the graphs given in all cases above are the only irreducible graphs of G which proves the last claim. \square

Proposition 5.10 draws a consequence of Theorem 5.3 and 5.9.

Proposition 5.10. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is regular and has at least one L-face. Let us apply the corresponding S^n -rules to G given in Table 1 to obtain a labeled cuboid graph $G'(V, E, \mathcal{F}')$. Then G' contains only one iso-path.*

Proof. The application of S^n -rule to G , where the S -rule is chosen according to Table 1, gives an irreducible graph G' . Hence, the irreducible graph G' has a single iso-path as proven in Theorem 5.9. The iso-path of G' is as well one of the inner iso-paths of G . \square

Proposition 5.11 draws a consequence of Theorem 5.3, 5.7 and 5.9.

Proposition 5.11. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be reducible. Then the successive application of one of the S -rules to G transforms G to an irreducible graph. Here the S -rule is chosen according to Table 1 if G has at least one L-face and, otherwise, the S -rule is chosen using the results given in Theorem 5.7.*

Proof. First, if G has at least one L-face we apply Proposition 5.10. Second, if G is L-face free, then if $D(G) = 2$ then apply once the S_1 -rule to G to get an irreducible graph G' with only one disperse node. In case $D(G) = 6$ apply once the S_3 -rule to G to get an irreducible graph G' with seven disperse nodes.

The second result follows by the arguments used to prove Theorem 5.7. \square

Proposition 5.12. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be regular. Suppose that the subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G is a regular face. Then there exists only one iso-path of G that passes through the iso-line on the regular face H if one of the following conditions is satisfied:*

- (a) G is irreducible,
- (b) G has no L -face,
- (c) G has one or more L -faces, but there is no subgraph $H(V_h, E_h, \mathcal{F}_h)$ of G such that $H \in [\hat{g}_2]_\circ$.

Proof. We consider two cases.

Case 1: If G is an irreducible graph then there exists exactly one iso-path in G and the iso-path passes through all iso-lines of regular faces of G as proven by Theorem 5.9.

Case 2: If G is reducible then we consider two subcases.

First, if G has no L -face then application of the S_1 -rule to G in case $D(G) = 2$ changes the disperse node on the face to a continuous node such that the resulting face is a continuous face. In case $D(G) = 6$ application of the S_3 -rule to G changes the continuous node on the face to a disperse node such that the resulting face is a disperse face. These results follow from the arguments used to prove Theorem 5.7 for the cases $D(G) = 2$ and $D(G) = 6$. Now, note that no iso-lines of G lie on disperse or continuous faces of G . Hence in both cases only one iso-path of G passes through the iso-line on the regular face H .

Second, if G has at least one L -face then application of one of the S -rules chosen according to Table 1 will decrease the number of L -faces of G and never create new L -faces. Hence, there exists only one iso-path of G that passes through the iso-line on the regular face H . This holds, because after computing an iso-path of G that passes through an iso-line on a regular face, then the number of disperse nodes of G that lie on the regular face increase or decrease. In case the number of disperse nodes on the regular face increases, then the resulting face is a disperse face or a singular face. But in case the number of disperse nodes of the regular face decreases, then the resulting face is a continuous face. Note that no iso-lines of G lie on singular faces of G . The arguments given in the second subcase follow from the arguments used to prove Theorem 5.3 for the cases $D(G) = 2$ to $D(G) = 6$. Hence, through the iso-line of a regular face H passes only one iso-path of G . \square

Proposition 5.13. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Assume G is regular and has at least one non-trivial L -face $H(V_h, E_h, \mathcal{F}_h)$. Let the S -rule that will be applied on G be chosen according to Table 1. If the S -rule that will be applied on G is either the S_1 - or S_2 -rule then there exist two iso-lines on H and to each iso-line there exists an inner iso-path of G that passes through it. If the S_3 -rule will be applied on G then one of the following holds:*

- (a) *in case H has no iso-nodes then there exist two iso-lines on H and to each iso-line there exists an iso-path of G that passes through it such that none of the iso-paths lies on the L-face.*
- (b) *in case one continuous node of H is an iso-node then there exists one iso-line on H and to the iso-line there exists an iso-path of G that passes through it such that the iso-path does not lie on the L-face.*

Proof. We consider two cases.

Case 1: Either the S_1 - or S_2 -rule will be applied on G . Then, applying Proposition 5.6 we find that through one of the iso-lines passes an iso-path of G . The S_1 - or S_2 -rule then changes the disperse node corresponding the iso-line to a continuous node. Then there remain only one disperse node on the face. Hence the L-face will be transformed to a regular face with only one disperse node. On a regular face lies only a single iso-line and through this iso-line passes only one iso-path of G according to Proposition 5.12. But H is a non-trivial L-face and, hence, both iso-paths passes through two different iso-lines on H and both iso-paths are different.

Case 2: The S_3 -rule will be applied on G . Then, applying Proposition 5.6 we find that through one of the iso-lines passes an iso-path of G . The S_3 -rule then changes one of the continuous nodes of H which is not an iso-node of H to a disperse node. Then there remains only one continuous node on the face. Hence, the L-face will be transformed to a regular face if H has no iso-node. On a regular face lies only a single iso-line and through this iso-line passes only one iso-path of G according to Proposition 5.12. In this case, H is a non-trivial L-face and, hence, both iso-paths passes through two different iso-lines on H and both iso-paths are different. But in case, H has iso-node then the L-face will be transformed to a singular face. But on a singular face lies no iso-line. Therefore, in this case, only one iso-path passes through an iso-line of the L-face H . \square

5.3 Outer Iso-path of a labeled cuboid graph

Until now we have not considered iso-paths on an L-face of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ which is regular and has at least one L-face. This section is devoted to compute outer iso-paths of G . As we know on each regular and on each trivial L-face of G lies only one iso-line and on a singular face of G lies no iso-line. Consequently, there is no iso-path on each of these faces of G . But on a non-trivial L-face of G we can have an iso-path if there exists a face-neighbored labeled cuboid graph $G'(V', E', \mathcal{F}')$ with iso-level c which is regular.

Let $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ be labeled cuboid graphs with iso-level $c \in (0, 1)$. Suppose that G_1 and G_2 are regular and face neighbors. Let

$H_1(V_{h_1}, E_{h_1}, \mathcal{F}_{h_1}) \subset G_1$ be a face of G_1 and $H_2(V_{h_2}, E_{h_2}, \mathcal{F}_{h_2}) \subset G_2$ be a face of G_2 such that $V_{h_1} = V_{h_2}$. Note that, if H_1 is an L-face of G_1 this does not mean that the face H_2 is an L-face of G_2 . Hence, if we have an iso-path in H_1 , this does not mean that we have an iso-path in H_2 . Hence, the node values of the common face of G_1 and G_2 can be different in case both H_1 and H_2 are not regular faces. All these claims will be proved in this section.

If H_1 is an L-face then we give a *graph-theoretical rule* to indicate if an iso-path on it exists. This graph-theoretical rule is used for the computation of iso-paths on L-faces in Section 5.4. The graph-theoretical rules depend on the type of the L-face of G_1 , on the type of the S -rule which will be applied on G_1 and is chosen according to Table 1, and on the type of the face H_2 of G_2 , and in case G_2 has at least one L-face then, in addition, from the type of the S -rule which will be applied on G_2 and is chosen according to Table 1.

Note: When needed we use in special cases \square -equivalence for a labeled cuboid graph with iso-level $c \in (0, 1)$ as given in Notation 2.

Theorem 5.14. *Let $G_1(V_1, E_1, \mathcal{F}_1)$, $G_2(V_2, E_2, \mathcal{F}_2)$ be labeled cuboid graphs with iso-level $c \in (0, 1)$. We assume that both G_1 and G_2 are face neighbors such that the common face $H(V_h, E_h, \mathcal{F}_h)$ is a non-trivial L-face. Furthermore, suppose that both G_1 and G_2 are regular. Let the S -rules that will be applied on G_1 and on G_2 be chosen according to Table 1. Assume that on G_1 the rules S_1 or S_2 apply and on G_2 the rule S_3 applies. Then there exists an iso-path in H . Furthermore, to each iso-line on H there exists only one inner iso-path that passes through the iso-line.*

Proof. Let $G_1 \in [(1)]_{\square}^*$ and $G_2 \in [(2)]_{\square}^*$ with the sketches (1) and (2) as shown in Figure 40. Then the L-face H is in $[(a)]_{\square}$ or in $[(b)]_{\square}$ as shown in Figure 40. In the case $H \in [(a)]_{\square}$, application of the S_1 - or S_2 -rule to G_1 gives a graph represented by the sketch (a1) of Figure 41. For the same case, application of the S_3 -rule to G_2 gives a graph represented by sketch (a2) of Figure 41. These graph operations transform H to a graph represented by the sketch (a') of Figure 41. This is shown by the graph-theoretical rule (A1) and by the sequence (A2) in Figure 41. Hence we get an iso-path on H . For the case $H \in [(b)]_{\square}$ we apply the same procedure to transform H to a graph represented by the sketch (b') of Figure 42. These procedures are shown by the graph-theoretical rule (B1) and by the sequence (B2) in Figure 42. Hence we get an iso-path on H .

The last claim holds true because to each disperse node in H there is a *corresponding* iso-path in G_1 (we get this using the S_1 - or S_2 -rule on G_1), and to the continuous node of H which is not an iso-node, there exists a corresponding iso-path in G_2 (we get this using the S_3 -rule on G_2). Here, the word "corresponding" is to be understood in the sense of Notation 3. \square

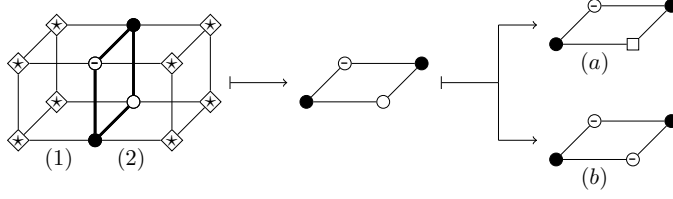


Figure 40: Sketches (1) and (2) represent $[(1)]_{\square}^*$ and $[(2)]_{\square}^*$. The common face of $G_1 \in [(1)]_{\square}^*$ and $G_2 \in [(2)]_{\square}^*$ is a non-trivial L-face. The sketches (a) and (b) represent $[(a)]_{\square}$ and $[(b)]_{\square}$ in which the two different types of non-trivial L-faces are obtained.

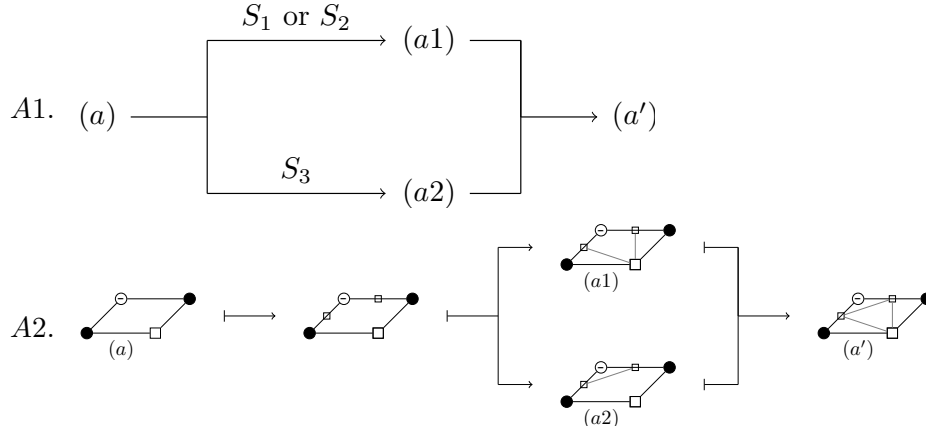


Figure 41: The graph-theoretical rule given by A1 and the sequence A2 illustrate the procedure how to compute an iso-path that lies on a non-trivial L-face which is in $[(a)]_{\square}$.

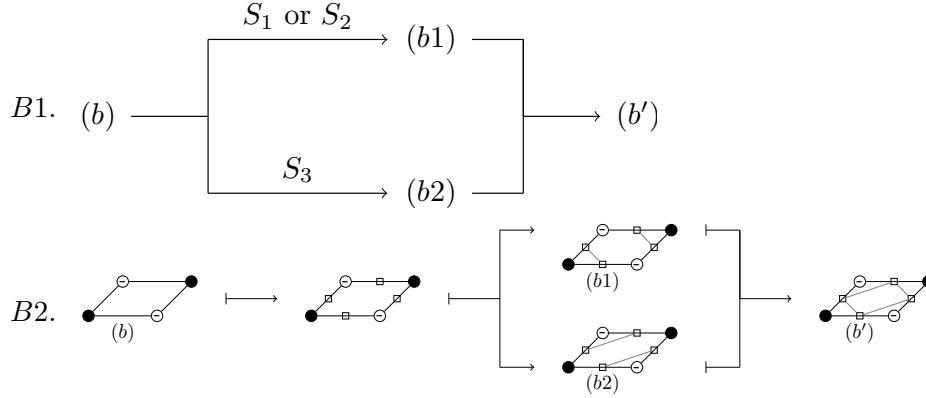


Figure 42: The graph-theoretical rule given by $B1$ and the sequence $B2$ illustrate the procedure to compute an iso-path that lies on a non-trivial L-face which is in $[(b)]_\square$.

Theorem 5.15. *Let $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ be labeled cuboid graphs with iso-level $c \in (0, 1)$. Assume that both G_1 and G_2 are face neighbors with a common L-face $H(V_h, E_h, \mathcal{F}_h)$. Furthermore, suppose that G_1 and G_2 are isolated iso-path free. Let $G_1 \in [(1)]_\square^*$ and $G_2 \in [(2)]_\square^*$, where the sketches (1) and (2) are as shown in Figure 43. Let the S -rules that will be applied on G_2 be chosen according to Table 1. Let one of the rules S_1 or S_2 be applicable on G_2 . Then there exists an iso-path in H . But if rule S_3 is applicable on G_2 then there exists no iso-path in H . Furthermore, to each iso-line on H there exists only one inner iso-path that passes through the iso-line.*

Proof. First, transform G_1 and G_2 to $G'_1(V_1, E_1, \mathcal{F}'_1)$ and $G'_2(V_2, E_2, \mathcal{F}'_2)$, respectively, by applying the T_1 -rule to each of them. Then we have $G'_1 \in [(1')]_\square^*$ and $G'_2 = G_2$, where sketch (1') is as shown in Figure 43. Then $H \subset G_1$ will be transformed to a graph in $[(a)]_\square$ and $H \subset G_2$ will be transformed to a graph in $[(b)]_\square$, with sketches (a) and (b) from Figure 43. We then apply the C_3 -rule to G'_1 and one of the rules S_1 or S_2 to G_2 in order to compute the iso-path on H as shown in sketch (c) of the sequence A2 of Figure 44. This procedure is illustrated by the graph-theoretical rule given by A1 in Figure 44.

The last claim holds true because to each disperse node in H there is a *corresponding* iso-path in G_2 (we get this using the S_1 - or S_2 -rule on G_2), and to the continuous node of H which is not an iso-node, there exists a corresponding iso-path in G_1 only if the S_3 -rule is applied on G_1 . Here, the word "corresponding" is to be understood in the sense of Notation 3. \square

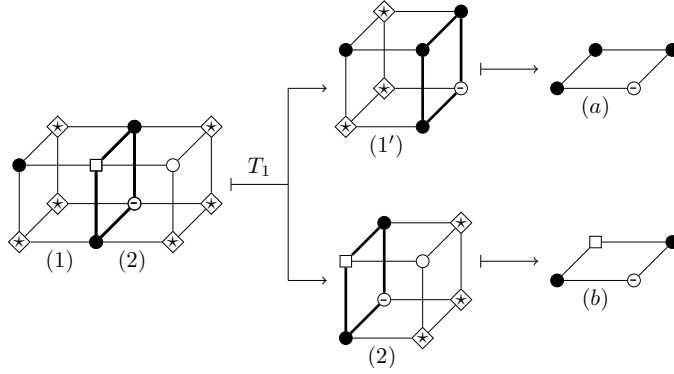


Figure 43: The sketches (1) and (2) represent $[(1)]_{\square}^*$ and $[(2)]_{\square}^*$, respectively. Sketches (a) and (b) represent faces of $G'_1 \in [(1')]_{\square}^*$ and $G_2 \in [(2)]_{\square}^*$, respectively. Both faces (a) and (b) have the same nodes, but different node weights.

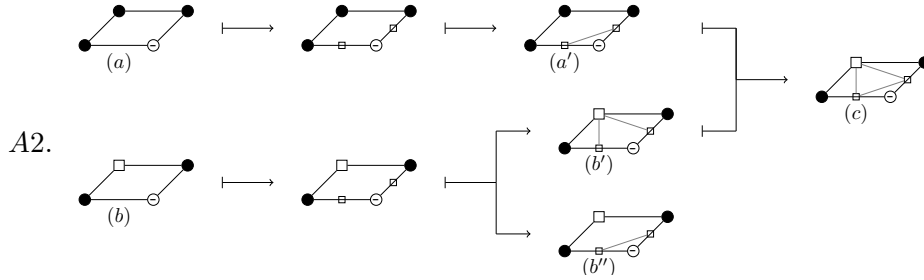
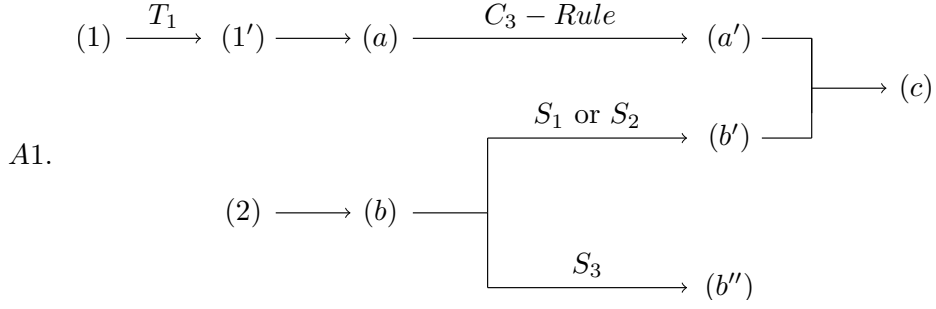


Figure 44: The graph-theoretical rule given by A1 and the sequence A2 illustrate the procedure to compute an iso-path that lies on a non-trivial L-face which is in $[(b)]_{\square}$.

Explanation of Figure 44 : The graph-theoretical rule A1 together with the sequence of the sketches A2 means that we first apply the T_1 -rule to G_1 , obtaining G'_1 . Then we apply to the common face of G'_1 and G_2 the C_3 -rule to get (a') . By applying the S_1 - or S_2 -rule to G_2 , we get $(b) \longrightarrow (b')$. But if

we apply the S_3 -rule to G_2 we get $(b) \longrightarrow (b'')$. From (b') we get an iso-path on the common face of G'_1 and G_2 . The sequence $A2$ in Figure 44 shows that the regular face obtained in $[(a)]_\square$ and the L-face obtained in $[(b)]_\square$ have iso-lines as shown by (a') and (b') or (b'') , respectively. In case (b') , the common face of G'_1 and G_2 has an iso-path as shown by (c) . In case (b'') , there is no iso-path on the common face of G'_1 and G_2 .

5.4 Algorithm for Complete Iso-path Computation

In this section we will give an algorithm for the complete iso-paths computation of a labeled cuboid graph $G(V, E, \mathcal{F})$ with iso-level $c \in (0, 1)$ which is neither disperse nor continuous.

The complete iso-paths of G will be computed in three steps. In the first step we delete all singular iso-paths or an isolated iso-path of G . These deletions will be carried out by transforming the graph G to a graph G' . If G' is regular then the second and the third step will be to compute the iso-paths of G' which are as well iso-paths of G . The only difference between the iso-paths of G and G' is that G' contains no singular iso-paths and no isolated iso-path. Here, if $D(G') \leq 7$ then G' is regular but if $D(G') = 8$ then G contains only singular or isolated iso-paths. In this case G' is a disperse labeled cuboid graph and has no iso-path and hence G has as well no iso-path. This means, in case G' is a disperse graph we consider as well G as a disperse graph.

Let $\Omega \subset \mathbb{R}^3$ be a polygonal domain allowing a partition into cuboids, i.e. $\bar{\Omega} = \cup_{i=1}^N C_i$ for the partition $\mathcal{T} = \{C_i\}_{i=1}^N$. Let $\mathcal{G} = \{G_1, \dots, G_N\}$ be a set of labeled cuboid graphs with common iso-level $c \in (0, 1)$, and let C_i be the cuboid of G_i for $i = 1, \dots, N$. The following algorithm computes the complete iso-paths of G_i for $i = 1, \dots, N$.

Algorithm for Iso-paths Computation

Notations: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Denote by $D(G)$ the total number of disperse nodes of G and by $L(G)$ and $L_{NT}(G)$ the set of L-faces and non-trivial L-faces of G , respectively. Recall the T_1^* -mapping as defined in Definition 4.7.

For $i = 1, \dots, N$ **do:**

Step 1: removing singular iso-paths or isolated iso-path

- i) removing singular iso-paths if $G_i = F_2(F_1(G_i))$:
 - a) $G'_i := T_2(T_1^*(G_i))$
 - b) if $(D(G'_i) = 8)$ then no iso-path, $i := i + 1$, **go to** Step 1
- ii) removing isolated iso-path if $G_i = T_2(T_1(G_i))$:
 - a) $G'_i := F_2(F_1(G_i))$

b) if $(D(G'_i) = 8)$ then no iso-path, $i := i + 1$, **go to** Step 1

Step 2: iso-path computation of G'_i for the case $L(G'_i) \neq \emptyset$

- (i) register all L-faces:
 let $L(G'_i) = \{\mathcal{L}_1, \dots, \mathcal{L}_l\}$ and $l = |L(G'_i)|$
- (ii) register all non-trivial L-faces of G'_i if $L_{NT}(G'_i) \neq \emptyset$:
 let $L_{NT}(G'_i) = \{\mathcal{M}_1, \dots, \mathcal{M}_m\}$ and $m = |L_{NT}(G'_i)|$
- (iii) let $\mathcal{N}_j \subset \mathcal{G}$ for $j = 1, \dots, m$ be all face neighbors of G'_i such that
 the common nodes of G'_i and \mathcal{N}_j are the nodes of \mathcal{M}_j
- (iv) use Table 1 to get the type of the S^n -rule corresponding to G'_i
 - a) use S^n -rule to compute iso-paths of G'_i
 $G''_i := S^n(G'_i)$
 Note: G''_i is the rest graph of G'_i and hence irreducible
 - b) use C -rules to compute the iso-path of G''_i (see Theorem 5.3)
- (v) **if** $m > 0$ **then** compute iso-path on non-trivial L-faces of G'_i :
 for $j = 1, \dots, m$
 - a) use Table 1 to get the type of the S -rule corresponding to \mathcal{N}_j
 - b) use Theorems 5.14 and 5.15 to compute a possible iso-path on \mathcal{M}_j

Step 3: iso-path computation of G'_i for the case $L(G'_i) = \emptyset$

if $D(G'_i) \in \{2, 6\}$ **and if** there exists H' in $[g_1]_\circ$ or in $[g_3]_\square$, **where**
 $H' \subset G'_i$, use Theorem 5.7 to compute iso-path
else
 apply C -rules to compute iso-path
endif

Note that the complexity of this algorithm is $O(N)$.

5.5 Application

Tracking or capturing interfaces of two-phase systems is an important issue for instance in computational fluid dynamics simulations [12]. The interfaces are used not only to track the phases but there can be adsorbed quantities on them like surfactants as well, which affect the hydrodynamics of the system [2]. Two well-known volume tracking methods are the Volume of Fluid (VOF) method [5] and the Level Set method [10]. The Level Set method uses a signed distance function which implicitly determines the interface as the zero level set. While level set methods are advantageous concerning discrete mean curvature computation, they suffer from volume loss of the disperse phase. The latter requires reinitialization of the level set function which introduces non-physical changes. The VOF-method conserves the phase volumes, but the standard interface reconstruction using a piecewise planar approximation (PLIC, [11]) leads to disconnected interface representations.

The present iso-surface algorithm can be employed to obtain a connected interface approximation instead.

Consider a polygonal domain $\Omega \subset \mathbb{R}^3$ and a domain partition $\mathcal{T} = \{C_i\}_{i=1}^N$ of $\bar{\Omega}$ into cuboids. Given a function $v : \mathcal{T} \rightarrow [0, 1]$ which gives the volume fractions of one of the phases (say the disperse phase), we define a labeling function $\mathcal{F} : \mathcal{P} \rightarrow [0, 1]$, where \mathcal{P} is the set of vertices of all cuboids in \mathcal{T} , by

$$\mathcal{F}(P) = \frac{1}{|I_P|} \sum_{i \in I_P}^n v(C_i), \quad (34)$$

where $i \in I_P$ if and only if $P \in C_i$. Using the labeling function \mathcal{F} , we get from $\mathcal{T} = \{C_i\}_{i=1}^N$ labeled cuboid graphs $G_1(V_1, E_1, \mathcal{F}_1), \dots, G_N(V_N, E_N, \mathcal{F}_N)$. Next, we interpolate the node values onto the edges according to Definition 2.1. Then, for a given $\epsilon > 0$, we determine for all graphs G_1, \dots, G_N a common iso-level $c \in (0, 1)$ by solving the inequality

$$\left| 1 - \frac{\Omega_D(c)}{\sum_{i=1}^N v(C_i)|C_i|} \right| < \epsilon, \quad (35)$$

where the domain $\Omega_D(c) \subset \mathbb{R}^3$ is the union of all bounded volumes enclosed by the iso-surface for the given iso-level c . Note that $\Omega_D(c)$ contains all disperse nodes of G_1, \dots, G_N .

The function $\gamma : [0, 1] \rightarrow (-\infty, \infty)$ given by

$$\gamma(c) = 1 - \frac{\Omega_D(c)}{\sum_{i=1}^N v(C_i)|C_i|} \quad (36)$$

measures the deviation between the total volume of the given disperse phase and that of the computed enclosed volume. The function γ is decreasing, but not necessarily strictly decreasing. Furthermore, γ can have (small) jumps. The latter can appear at an iso-level c if \mathcal{F} attains the value c on several, complete edges. In such cases, the error bound ϵ in (35) cannot be chosen arbitrarily small.

Using the iso-surface algorithm from Section 5.4 we first computed iso-surfaces for snap shots of the simulated collision of two liquid droplets. The snap shots are taken at different time steps and the resulting iso-surfaces are shown in Figure 45. We have also applied the iso-surface algorithm to the outcome of a crown splash, where one typical snap shot is shown in Figure 46. For the iso-surface computation of the binary droplet collision and the splash we computed the iso-level c using $\epsilon = 10^{-9}$ in (35).

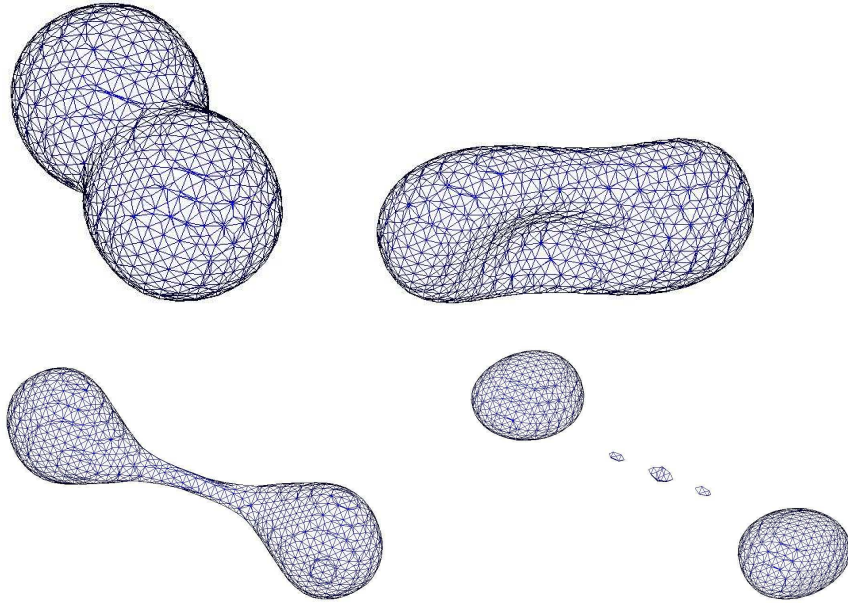


Figure 45: The sequence of sketches show iso-surface meshes for snap shots of a boundary droplet collisions taken at different time steps.

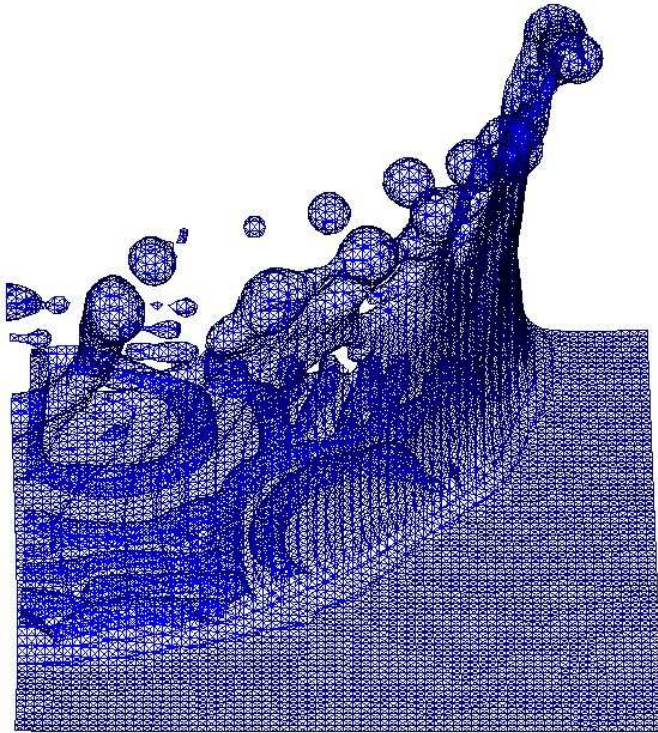


Figure 46: The figure shows the iso-surface mesh for a snap shot of a crown splash.

The highly dynamic impact of a droplet into a liquid layer which produces the crown-splash is a good validation example, since during the splash several special cases occur in the iso-surface computation. Indeed, there appear labeled cuboid graphs $G(V, E, \mathcal{F})$ containing

1. singular faces,
2. a trivial L-face,
3. non-trivial L-faces,
4. edges with iso-node end points.

Sketches (a1), (a2) and (a3) of Figure 47 illustrate some of the special cases which appear. Sketch (a1) illustrates a labeled cuboid graph and its iso-path, where the graph contains a singular face. Sketch (a2) illustrates a labeled cuboid graph and its iso-path, where the graph contains a trivial L-face. Sketch (a3) illustrates a labeled cuboid graph and its iso-path, where the graph contains two non-trivial L-faces and an edge with iso-nodes as end points of it.

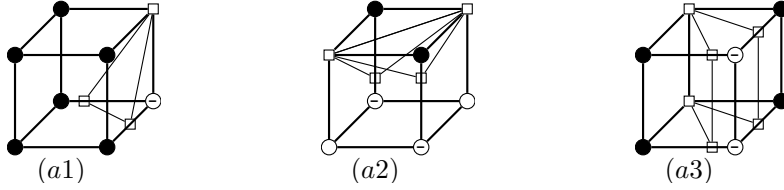


Figure 47: Sketches (a1), (a2) and (a3) illustrate labeled cuboid graphs and their iso-paths, where each of the cuboids has at least one iso-node.

6 Connectedness of Iso-paths

Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Then an iso-line in G can be common for two distinct iso-paths that lie in G . In all other cases an iso-line in G can be common for at least two iso-paths, one corresponding to G and one or more corresponding to another labeled cuboid graph $G'(V', E', \mathcal{F}')$, where G' is a face or edge neighbor of G . Iso-lines which are common for at least two iso-paths are as well common for the corresponding iso-elements. Therefore, a common iso-line of at least two iso-paths is common for at least two distinct iso-elements. This means that iso-elements are connected via such iso-lines. We also say that the iso-paths are connected at the common iso-line. If each edge of an iso-path is common for at least two distinct iso-paths then we say that

the iso-path is connected. Connected iso-paths give rise to connected iso-surfaces. Therefore, connectedness of iso-paths is a very important property which will be investigated in this section.

Consider a polygonal domain $\Omega \subset \mathbb{R}^3$ having a cuboid partition $\mathcal{T} = \{C_i\}_{i=1}^N$ such that $\overline{\Omega} = \cup_{i=1}^N C_i$. Let $\mathcal{G} = \{G_1, \dots, G_N\}$ be a set of labeled cuboid graphs with common iso-level $c \in (0, 1)$ and C_i be the cuboid of G_i for $i = 1, \dots, N$. We compute the iso-paths in each G_i by applying the algorithm given in Section 5.4. Then the following questions arise:

1. is it possible to show iso-surface connectivity?
2. is it possible to decompose iso-surfaces into components such that each edge of an iso-element in a component is a common to only two distinct iso-elements in the same component?
3. how to compute discrete mean curvature at iso-points?
4. is it possible to get all local topological information of an iso-surface in a simple way?

The first problem will be answered affirmative in this section and the remaining questions will receive a positive answer in Sections 7 and 8.

Note: When needed we use in special cases \square -equivalence for a labeled cuboid graph with iso-level $c \in (0, 1)$ as given in Notation 2.

Theorem 6.1. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Suppose G is regular and has a trivial L-face. Then G contains exactly two distinct inner iso-paths. Furthermore, G has only one trivial L-face.*

Proof. It holds that $G \in [(a)]_{\square}$ or $G \in [(b)]_{\square}$ or $G \in [(c)]_{\circ}$, where the sketches (a) , (b) , (c) are as given in Figure 48, since precisely in these cases G is isolated iso-path free. We then apply the S_1^2 -rule to G if $G \in [(a)]_{\square}$, or apply S_1 - and S_2 -rules to G if $G \in [(b)]_{\square}$, or apply the S_2^2 -rule to G if $G \in [(c)]_{\square}$. We get in all cases two distinct inner iso-paths in G . Furthermore, if $G \in [(d)]_{\square}$ then application of the F_1 -rule to G transforms G to a labeled cuboid graph $G'(V, E, \mathcal{F}') \in [(e)]_{\square}$ where the sketches (d) and (e) are as given in Figure 48. But G' is a disperse graph and has no L-faces. Hence, G has only one trivial L-face. \square

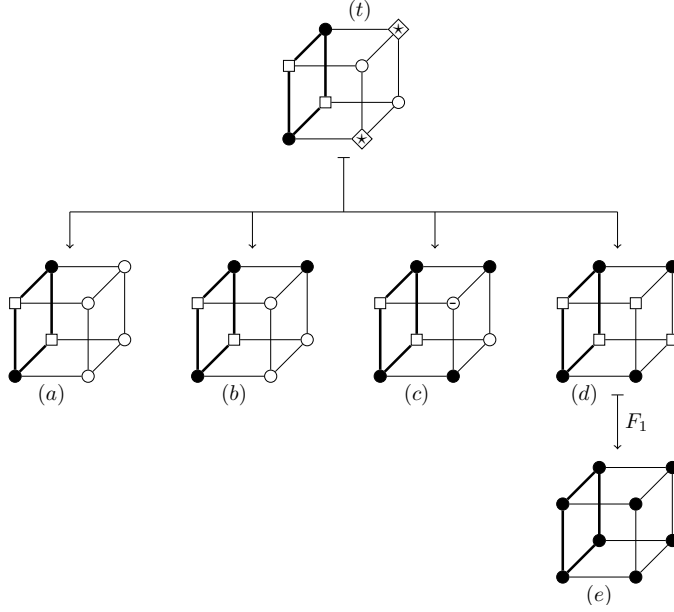


Figure 48: Sketch (t) represents $[(t)]_{\square}^*$. Then, by substituting in (t) for the unknowns of the two nodes marked by the symbol \diamond the symbols \circ or \bullet , we get four different types of labeled cuboid graphs that lie in $[(a)]_{\square}$, $[(b)]_{\square}$, $[(c)]_{\square}$ or $[(d)]_{\square}$, respectively.

Lemma 6.2. *Let $G_1(V_1, E_1, \mathcal{F}_1)$ and $G_2(V_2, E_2, \mathcal{F}_2)$ be labeled cuboid graphs with iso-level $c \in (0, 1)$. We assume that both G_1 and G_2 are face neighbors with a trivial L-face $H(V_h, E_h, \mathcal{F}_h)$. Furthermore, suppose that G_1 and G_2 are isolated iso-path free. Then there exist exactly two distinct inner iso-paths in G_2 that pass through the iso-line in H .*

Proof. We consider two different labelings of $G_1 \in [(1)]_{\square}^*$ and $G_2 \in [(2)]_{\square}^*$ as given by the graphical sequences in A and B of Figure 49. Transform first G_1 and G_2 to $G'_1(V_1, E_1, \mathcal{F}'_1)$ and $G'_2(V_2, E_2, \mathcal{F}'_2)$, respectively, by applying the T_1 -rule to each of them. Then we have $G'_1 \in [(1')]_{\square}^*$ and $G'_2 = G_2$, where sketch $(1')$ is as shown in Figure 49. Furthermore, the common trivial L-face of graphs G_1 and G_2 will be transformed to $H_1(V_h, E_h, \mathcal{F}_h) \in [(a)]_{\square}$ and to $H_2(V_h, E_h, \mathcal{F}_h) \in [(b)]_{\square}$, respectively. Sketches (a) and (b) are as shown in Figure 49. Both G'_1 and G_2 are isolated iso-path free and, hence, there exists an iso-path in G_2 . But since we have a trivial L-face in G_2 , we have at least two distinct inner iso-paths in G_2 that pass through the iso-line in H according to Theorem 6.1. Application of S_1^2 - or S_2^2 -rule or S_1 - and S_2 -rules to $G_2 \in [(2)]_{\square}$, where G_2 is isolated iso-path free, we get exactly two distinct inner iso-paths of G_2 . \square

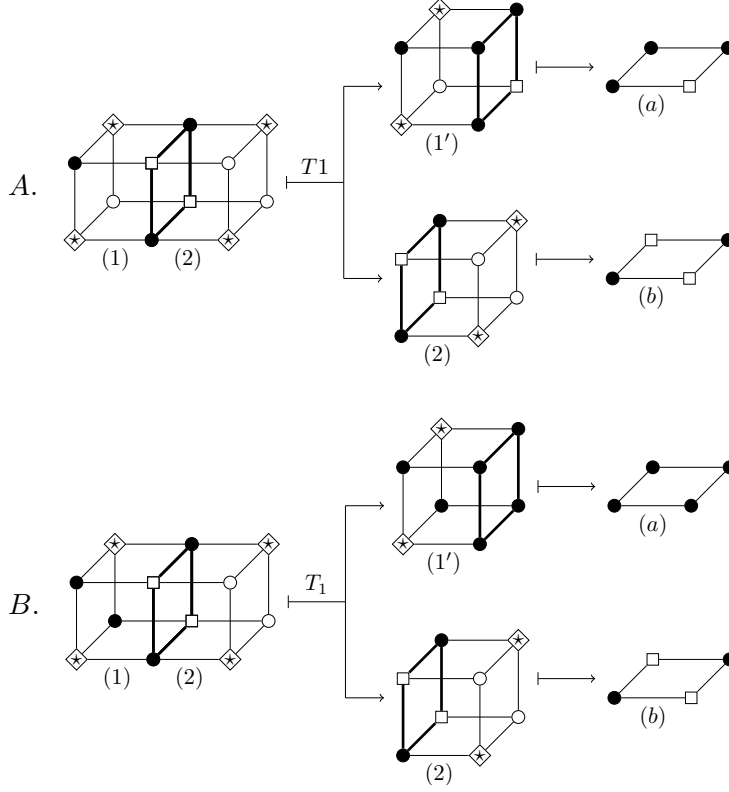


Figure 49: Application of T_1 -rule to $G_1 \in [(1)]_{\square}^*$ and to $G_2 \in [(2)]_{\square}^*$ transforms the common trivial L-face of both graphs to graphs in $[(a)]_{\square}$ and in $[(b)]_{\square}$, respectively. The sequences of sketches A and B show the complete possible results.

Theorem 6.3. *Let $G_1(V_1, E_1, \mathcal{F}_1) \in [(1)]_{\square}^*$ and $G_2(V_2, E_2, \mathcal{F}_2) \in [(2)]_{\square}^*$ with iso-level $c \in (0, 1)$ where sketches (1) and (2) are as shown in Figure 50. Both G_1 and G_2 are face neighbors with a regular face $H(V_h, E_h, \mathcal{F}_h)$ which is in $[(a)]_{\circ}$ or $[(b)]_{\square}$ or $[(c)]_{\square}$, where sketches (a), (b), (c) are as shown in Figure 51. Then there is only one iso-line in H .*

Proof. Apply the C -rules to H . We consider in Figure 50 different labelings of G_1 and G_2 which give different types of regular faces as a face neighbor of both graphs. In all these cases as shown by the graphical sequences A , B and C in Figure 50 we get, by applying the C -rules to each of the regular faces, a single iso-line. \square

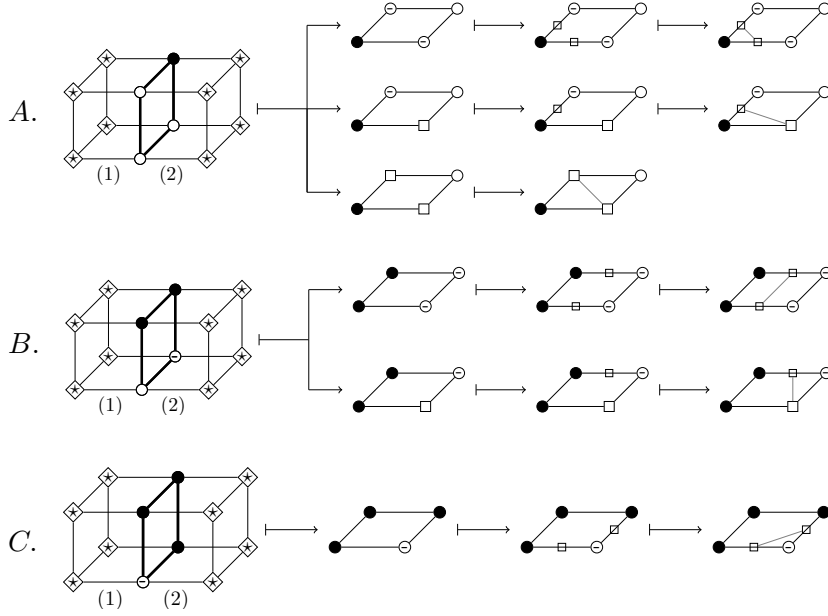


Figure 50: The sequences A , B , and C show that for a common regular face of $G_1 \in [(1)]_{\square}^*$ and $G_2 \in [(2)]_{\square}^*$ we get an iso-line on the common face on G_1 as well as on G_2 as shown in the last sketch of each sequence.

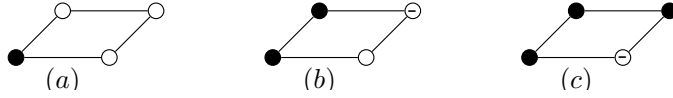


Figure 51: Regular faces of one, two and three disperse nodes. Each of the regular faces of two and three disperse nodes has at least one non-iso-node.

Lemma 6.4. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let $G \in [(a)]_{\square}$, where the sketch (a) is as shown in Figure 52. Then G contains exactly two distinct inner iso-paths. Both iso-paths pass through the edge e of the graph G .*

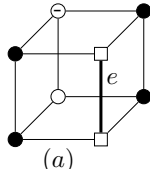


Figure 52: Sketch (a) illustrates $G(V, E, \mathcal{F}) \in [(a)]_{\square}$. The edge e of G has two iso-node end points.

Proof. Apply the S_2^2 -rule to G . □

Proposition 6.5. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Suppose G is regular. Let G have two iso-points which are iso-nodes that lie on the same edge of a cuboid of G . Then the maximum number of distinct iso-paths that pass through both iso-nodes is two.*

Proof. According to Lemma 6.4 any graph in $[(a)]_\square$, where sketch (a) is as shown in Figure 52, has two distinct iso-paths that pass through both iso-nodes. The maximum number of inner iso-paths that passes through two iso-points which are iso-nodes and are end points of an edge of G is attained only if $G \in [(a)]_\square$. \square

Definition 6.6. *(System of cuboids and system of labeled cuboid graphs at an edge). Let C_1 be a cuboid with vertices P_1, \dots, P_8 . Let $e = \overline{P_1 P_2}$ be an edge of C_1 . Then let C_2, C_3, C_4 be distinct cuboids such that C_i for $i = 1, \dots, 4$ have the edge e in common and if $C_i \cap C_j \not\subseteq e$ for $i \neq j$ then C_i and C_j have a common face. Then we say C_1, \dots, C_4 are the system of cuboids with common edge e . Furthermore, let $G_i(V_i, E_i, \mathcal{F}_i)$ for $i = 1, \dots, 4$ be labeled cuboid graphs with a common iso-level $c \in (0, 1)$ and be singular iso-path free and isolated iso-path free. In addition, let C_i be the cuboid of G_i for $i = 1, \dots, 4$. Then we say G_1, \dots, G_4 are the system of labeled cuboid graphs with common edge e .*

The following lemma is a direct geometrical consequence of Definition 6.6.

Lemma 6.7. *Let C_i and $G_i(V_i, E_i, \mathcal{F}_i)$ for $i = 1, \dots, 4$ be a system of cuboids and a system of labeled cuboid graphs, respectively, corresponding to the common edge e such that C_i is a cuboid of G_i . Then to each cuboid $C \in \{C_1, \dots, C_4\}$ there exist two distinct cuboids C_i and C_j in $\{C_1, \dots, C_4\}$ such that C and C_i as well as C and C_j have a common face. Analogously, to each labeled cuboid graph $G \in \{G_1, \dots, G_4\}$ there exist two distinct graphs G_i and G_j in $\{G_1, \dots, G_4\}$ such that G and G_i as well as G and G_j are face neighbored.*

Theorem 6.8. *Let C_i and $G_i(V_i, E_i, \mathcal{F}_i)$ for $i = 1, \dots, 4$ be a system of cuboids and a system of labeled cuboid graphs, respectively, corresponding to the common edge e such that C_i is a cuboid of G_i . Let $e = \overline{P_1 P_2}$ and assume that the nodes of G_1 corresponding to the end points of e are iso-nodes ($\mathcal{F}_1(P_1) = \mathcal{F}_1(P_2) = c$), where $c \in (0, 1)$ is the common iso-level of G_i for $i = 1, \dots, 4$. Let the total number of iso-paths that pass through e be denoted by $N(e)$. Then $N(e) \in \{0, 2m\}$, where $m \leq 4$. If $m \geq 1$, denote the iso-paths by $\omega_1, \dots, \omega_{2m}$. Additionally, denote by G_{ω_i} the labeled cuboid graph corresponding to ω_i and by C_{ω_i} the cuboid of G_{ω_i} for $i = 1, \dots, 2m$. If $m \geq 1$ then to any $\omega \in \{\omega_1, \dots, \omega_{2m}\}$ there exists $\omega' \in \{\omega_1, \dots, \omega_{2m}\}$, $\omega' \neq \omega$, such that one of the following holds:*

- (i) G_ω and $G_{\omega'}$ are face neighbored and have two common disperse nodes,

(ii) if (i) does not hold then $m \leq 3$ and there exists a unique $l \in \{1, \dots, 4-m\}$ which depends on ω and ω' such that G_ω is face neighbored to G_{r_1} and G_{r_l} is face neighbored to $G_{\omega'}$, where $\{G_{r_1}, G_{r_l}\} \subset \{G_1, \dots, G_4\}$. Furthermore, if $l > 1$ then G_{r_i} is face neighbored to $G_{r_{i+1}}$ for $i = 1, \dots, l-1$. In addition, each G_{r_i} for $i = 1, \dots, l$ has at least seven disperse nodes and, hence, they have no iso-path that passes through e . Note that for $l = 1$ it holds $G_{r_1} = G_{r_l}$.

Then we say the pair ω and ω' are disperse connected with respect to the common iso-line e . Furthermore, this property is unique and, hence, there is no other iso-paths which are disperse connected either to ω or ω' with respect to e .

Note that all graphs and cuboids stated above are in the system of labeled cuboid graphs and in the system of cuboids corresponding to the edge e , respectively.

Proof. The proof will be given using the following two parts.

1. Uniqueness of disperse connectivity of ω and ω' with respect to e .

If this is not the case, then either G_ω or $G_{\omega'}$ has an additional disperse node and there exists a graph $G \in \{G_1, \dots, G_4\}$, where $G \not\subset \{G_{r_1}, G_{r_l}\}$ such that G is either face neighbored to G_ω or to $G_{\omega'}$ and G is disperse or G contains no iso-path that passes through e . If G is not disperse but has no iso-path that passes through e then G contains seven disperse nodes (this follows from the application of T_2 -rule to G). But in this case the face neighbored graph to G , which is G_ω or $G_{\omega'}$, has two additional disperse nodes in common with G . Then either G_ω or $G_{\omega'}$ has at least five disperse nodes. But then application of T_2 -rule to the graph with at least five disperse nodes leads to a labeled cuboid graph with seven disperse nodes. Then the graph will have no iso-path that passes through e . But this is a contradiction to the regularity of G_ω and $G_{\omega'}$. This proves the claim for the unique disperse connectivity of ω and ω' .

2. Proof validity of cases (i) and (ii).

Let us assume that an iso-path ω exists in G_ω such that the iso-path passes through e . Then G_ω is regular and, hence, G_ω has at least two disperse nodes. From Lemma 6.7 we know that it is possible to rename the graphs G_1, \dots, G_4 such that G_i is face neighbored to G_{i+1} for $i = 1, \dots, 3$ and G_4 is face neighbored to G_1 . Now the proof follows using the following two steps:

Step 1. Since G_ω is regular there exists a face neighbor $G \in \{G_1, \dots, G_4\}$ to G_ω such that G and G_ω have two common disperse nodes corresponding to e . If G is regular and has an iso-path that passes through e then case (i) is satisfied.

Step 2. But if G given in Step 1 has no iso-path that passes through e then from the application of T_2 -rule to G we get \tilde{G} , where \tilde{G} has at least seven disperse nodes. Then \tilde{G} has no iso-path that passes through e . But since all graphs G_1, \dots, G_4 are singular iso-path free and isolated iso-path free we have $G = \tilde{G}$. Again G is face neighbored with $G' \in \{G_1, \dots, G_4\}$ such that $G' \notin \{G, G_\omega\}$. Hence, G' and G have at least two disperse nodes in common. If G' is regular and has an iso-path that passes through e then case (ii) is satisfied by choosing $G_{r_1} = G$. But if G' has no iso-path that passes through e then G' has at least seven disperse nodes (again after application of T_2 -rule to G'). Hence, in case G' has at least seven disperse nodes set $G_{r_2} := G'$, and $G := G'$ and then apply again Step 2 until case (ii) is satisfied.

Note that there exists a regular graph $G_{\omega'}$, disperse connected to G_ω with respect to edge e . If this is not the case, then each face neighbored graphs G_p and G_q of G_ω , where $\{G_p, G_q\} \subset \{G_1, \dots, G_4\}$ and $G_p \neq G_q$, have at least seven disperse nodes. Then G_q and G_ω have two common disperse nodes. But since G_p is face neighbored to G_ω and not face neighbored to G_q , G_p and G_ω have another two common disperse nodes. But then G_ω has at least four disperse nodes. Furthermore, there exist four disperse nodes of G_ω denoted by Q_1, Q_2, Q_3, Q_4 such that each P_1, P_2, Q_1, Q_2 and P_1, P_2, Q_3, Q_4 are face vertices of the cuboid of G_ω , where P_1, P_2 are the end points of e . Furthermore, there exists a graph G_s which is face neighbored with G_q and G_p . In addition, G_s has at least seven disperse nodes (this follows from the assumption that there exists no $G_{\omega'}$ which is disperse connected with G_ω). If G_ω is regular and has only four disperse nodes then application of Proposition 6.5 gives that G_ω has two iso-paths and both iso-paths passes through e and hence both iso-paths are disperse connected with respect to e ; therefore, case (ii) is satisfied. In this case, we use $G_{r_1} = G_p$, $G_{r_2} = G_s$, $G_{r_3} = G_q$ in (ii) of Theorem 6.8. But then in G_ω there exist two iso-paths ω and ω' which are disperse connected with respect to e . This is a contradiction to the assumption that there exists no ω' which is disperse connected to ω with respect to e . In case G_ω has five disperse nodes then application of T_2 -rule to G_ω gives that G_ω has at least seven disperse nodes and, hence, G_ω has no iso-path that passes through e . This is a contradiction to the assumption that G_ω has an iso-path that passes through e , hence this case does not occur. Consequently, case (ii) holds.

To conclude, the set of all iso-paths that pass through e can be uniquely decomposed into pairs such that each pair is disperse connected with respect to e . Hence, the total number of iso-paths in the system of graphs which

pass through e is an even number. The maximum number is 8 as follows from Proposition 6.5). \square

Theorem 6.9. (*Connectedness of iso-paths*). *Let the polygonal domain $\Omega \subset \mathbb{R}^3$ have a domain partition $\mathcal{T} = \{C_i\}_{i=1}^N$ into cuboids. Let $\mathcal{G} = \{G_1, \dots, G_N\}$ be a set of labeled cuboid graphs with common iso-level $c \in (0, 1)$, and C_i be the cuboid of G_i for $i = 1, \dots, N$. Assume that all G_i , $i = 1, \dots, N$, singular iso-path free and isolated iso-path free. Compute the complete iso-paths in each G_i by applying the algorithm given in Section 5.4. Then each iso-line of an arbitrary $G \in \mathcal{G}$ is common for at least two distinct iso-paths, where the iso-paths can be in G or in face- or in edge-neighbors of G .*

Proof. We prove the claim by distinguishing different cases:

Case 1: In case an iso-line l is an edge of $G \in \mathcal{G}$ then Theorem 6.8 says that we have at least two iso-paths in \mathcal{G} which have l as a common iso-line.

Case 2: In case an iso-line l lies on a trivial L-face of $G \in \mathcal{G}$, Theorem 6.1 says that we have two iso-paths in G which have l as a common iso-line. We even get four iso-paths with l as a common iso-line if the trivial L-face is common for G and G' , where $G' \in \mathcal{G}$ is a face neighbor of G .

Case 3: Let $H \subset G$ be a regular face of G . Assume that H is as well a face of $G' \in \mathcal{G}$, where G' is a face neighbor of G . Then Proposition 5.12 implies that each of the graphs G and G' contains exactly one inner iso-path running through l .

Case 4: Let an iso-line l lie on a non-trivial L-face $H(V_h, E_h, \mathcal{F}_h)$ of $G \in \mathcal{G}$. Then we consider two subcases:

(a) Suppose H is a common non-trivial L-face of G and $G'(V', E', \mathcal{F}') \in \mathcal{G}$. Then one of the following holds:

- (i) if there exists an iso-path on each of the L-faces then each iso-line on the L-face is part of an iso-path that does not lie on the L-face as shown in Proposition 5.13. Therefore, to each iso-line there exist two iso-paths, where the first iso-path is an inner iso-path and the second iso-path is the iso-path on the L-face.
- (ii) if there exists no iso-path on each of the L-faces then Proposition 5.13 says that to each iso-line on the L-face there exists an iso-path in G and in the face neighboring graph. Hence to each iso-line on the L-face there exist two iso-paths.

(b) Suppose $G'(V', E', \mathcal{F}') \in \mathcal{G}$ is a face neighbor of G , where $H'(V'_h, E'_h, \mathcal{F}'_h)$ is a regular face of G' and $V_h = V'_h$. Then one of the following holds:

- (i) if there exists an iso-path on the L-face then we have the same conclusion as in (i) of (a).
- (ii) if there exists no iso-path on the L-face then we have the same conclusion as in (ii) of (a). \square

7 Components of iso-surfaces

In this section we show how to compute separate components of connected iso-surfaces such that on each component normals and discrete mean curvature can be calculated. We give definitions required to define iso-path connectivity such that an iso-surface can be decomposed into its components. These components are orientable and connected.

We have proved in Section 6 using Theorem 6.9 that the iso-surfaces computed by applying the algorithm given in Section 5.4 are connected. This means to each iso-line l of an iso-path there exist at least two iso-paths such that l is a common edge to them. Theorem 6.8 and Theorem 6.1 show that an iso-line l can be common for up to eight or four iso-paths, respectively. It is clear that discrete mean curvature computation at the end points of l , where l is common to more than two iso-paths, is not defined. Hence, we will give a definition which allows to decompose the iso-surfaces into connected components such that at each iso-point of the connected components discrete mean curvature computation is possible.

To define components of closed iso-surfaces we need the notion of a *disperse path* which is a simple path but not a loop such that it consists solely of edges of cuboids which only have disperse nodes as end points. Such a path runs within the *system of graphs*, which is defined next.

Definition 7.1. (*System of cuboids and system of graphs*). Let C be a cuboid with vertices P_1, \dots, P_8 and edges e_1, \dots, e_{12} . Then let C_1, \dots, C_{12} be the system of cuboids (see Definition 6.6) with respect to edges e_1, \dots, e_{12} , respectively. For each $i = 1, \dots, 12$ and $j = 1, \dots, 4$ we denote by C_{ij} the cuboids such that

$$C_i = \{C_{ij} : j = 1, \dots, 4\} \text{ for } i = 1, \dots, 12,$$

where $C = C_{i1}$ for all $i = 1, \dots, 12$, and the following holds:

- for all $x \in \{P_1, \dots, P_8\}$ there exists a neighborhood $U \subset \mathbb{R}^3$ of x such that $U \subset \cup_{i=1}^{12} \cup_{j=1}^4 C_{ij}$ and any two distinct cuboids in the set $\{C_{ij} : i = 1, \dots, 12 \text{ and } j = 1, \dots, 4\}$ have a common edge or a common face.

Then we say $C = C_{i1}$ and C_{ij} for $i = 1, \dots, 12$, $j = 2, \dots, 4$ are the system of cuboids of C . Furthermore, let $G_{i1}(V_{i1}, E_{i1}, \mathcal{F}_{i1})$ and $G_{ij}(V_{ij}, E_{ij}, \mathcal{F}_{ij})$ for $i = 1, \dots, 12$, $j = 2, \dots, 4$ be labeled cuboid graphs with a common iso-level

$c \in (0, 1)$ and singular iso-path free and isolated iso-path free. In addition, let C_{i1} and C_{ij} be the cuboids of G_{i1} and G_{ij} for $i = 1, \dots, 12$, $j = 2, \dots, 4$, respectively. Then we say that G_{i1} and G_{ij} for $i = 1, \dots, 12$, $j = 2, \dots, 4$ are the system of labeled cuboid graphs of $G(V, E, \mathcal{F})$, where $G = G_{i1}$ for all $i = 1, \dots, 12$. Additionally, we call $N(G)$ the number of system of graphs of G which is given by

$$N(G) = \sum_{i=1}^{12} n_i - \sum_{l=1}^6 (|E_{F_l}| - 1) - (|E| - 1), \quad (37)$$

where $n_i = |C_i| = 4$ for $i = 1, \dots, 12$, $F = \{F_1, \dots, F_6\}$ is the set of faces of C , E_{F_l} is the set of edges of face F_l of C for $l = 1, \dots, 6$, and $|\cdot|$ denotes the number of elements in a set. It holds $|E_{F_l}| = 4$ for $l = 1, \dots, 6$ and $|E| = 12$. Hence, in the present case of cuboids, $N(G) = 19$.

The derivation of formula (37) is easy and is therefore left to the reader. Equation (37) can be even applied to arbitrary partition of a polygonal domain which has the form as given in Definition 7.1.

Definition 7.2. (*Disperse path*). Let ζ be a simple, but not closed path in the system of graphs of a given labeled cuboid graph $G(V, E, \mathcal{F})$. If there is $r \geq 2$ and to each $m = 1, \dots, r$ there exists $G'_m(V'_m, E'_m, \mathcal{F}'_m)$ in the system of graphs of G and a disperse edge l_m of G'_m such that ζ is of the form $\zeta = \cup_{m=1}^r l_m$, we call ζ a disperse path in the system of graphs of G .

Remark 7.3. In the following, when we say "corresponding nodes of an iso-line" or "corresponding iso-line of nodes", the word "corresponding" is to be understood in the sense of Notation 3. Furthermore, when we say "disperse node or nodes corresponding to iso-line l with respect to an iso-path", then it means that l is an edge of the iso-path and l corresponds to the disperse node or nodes.

Definition 7.4. (*Disperse connectedness of two iso-paths at a common edge*). Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let G be regular and l be an iso-line of G . Let ω_1 and ω_2 be two distinct iso-paths with $l = \omega_1 \cap \omega_2$, where ω_1 is one of the iso-paths of G and ω_2 is an iso-path in the system of graphs of G . We say that ω_1 and ω_2 are disperse connected with respect to the common edge l if one of the following holds:

1. ω_1 and ω_2 are the only iso-paths in the system of graphs of G such that $l = \omega_1 \cap \omega_2$,
2. ω_1 is an inner iso-path of G , ω_2 is an inner iso-path for one labeled cuboid graph in the system of graphs of G , and one of the following holds:

- (a) at least one of the disperse nodes corresponding to l is the same for the iso-line l with respect to ω_1 and ω_2 ,
- (b) there exist two distinct disperse nodes P_1 and P_2 in the system of graphs of G such that P_1 is a node of G and P_2 may not a node of G . The disperse nodes P_1 and P_2 correspond to l with respect to ω_1 and ω_2 , respectively, and there exists a disperse path in the system of graphs of G which connects P_1 and P_2 .

We say that two distinct iso-elements Z_1 and Z_2 in the system of graphs of G are neighbored with respect to the iso-line $l = Z_1 \cap Z_2$ of G if the corresponding iso-paths ω_1 and ω_2 of Z_1 and Z_2 , respectively, are disperse connected with respect to l .

Convention of iso-elements disjointness: Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$. Let G be regular and l be an iso-line of G . Let Z_1 and Z_2 be two distinct iso-elements in the system of graphs of G which have l as a common iso-line ($l = Z_1 \cap Z_2$), but are *not* neighbored with respect to l . Then, concerning their connectivity, we consider both iso-elements Z_1 and Z_2 as disjoint. This means, given arbitrary points $P_1 \in Z_1$ and $P_2 \in Z_2$, there exists no path $\omega \subset Z_1 \cup Z_2$ that joins P_1 and P_2 . This convention helps to decompose iso-surfaces into connected components such that on each component computation of surface PDEs and discrete mean curvature is possible.

The next theorem will be used to decompose iso-surfaces into components.

Theorem 7.5. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be regular. Let ω be an iso-path of G , given by $\omega = [Q_1, Q_2, \dots, Q_n]$ with $n \geq 3$. We set $l_i = \overline{Q_i Q_{i+1}}$ for $i = 1, \dots, n-1$ and $l_n = \overline{Q_n Q_1}$ which are iso-lines of G and as well edges of ω . Then there exist iso-paths $\omega_1, \dots, \omega_n$ in the system of labeled cuboid graphs of G such that $l_i = \omega \cap \omega_i$ for $i = 1, \dots, n$ and each pair (ω, ω_i) is disperse connected with respect to l_i for $i = 1, \dots, n$.*

Proof. We prove the claim by considering three cases. In all these cases, we let $G'(V', E', \mathcal{F}')$ be a graph in the system of graphs of $G(V, E, \mathcal{F})$ such that G and G' are face-neighbored and the nodes of the face $H(V_h, E_h, \mathcal{F}_h)$ of G are common to both graphs G and G' . Suppose $H'(V'_h, E'_h, \mathcal{F}'_h) \subset G'$ is the face of G' such that $V'_h = V_h$.

Case 1: An iso-line $l \in \{l_1, \dots, l_n\}$ lies on a regular face $H(V_h, E_h, \mathcal{F}_h)$ of G .

We consider three subcases.

1. Assume that H contains only two disperse nodes and at least one of the continuous nodes is not an iso-node. Then the following holds:

- (a) $H = H'$.
- (b) An iso-line on H is common only for two iso-paths. The first iso-path lies in G and the second in G' . This follows from Proposition 5.12. The common iso-line of both iso-paths corresponds to the disperse nodes of H (cf. Remark 7.3).

Hence, condition 1 of Definition 7.4 is satisfied.

- 2. H has two disperse nodes and two iso-nodes. Then the following holds:
 - (a) If l is common for G and G' and if there exists an iso-path ω' in G' that passes through l such that the corresponding disperse nodes of ω and ω' with respect to l are the same, then both iso-paths are disperse connected.
 - (b) The other cases are shown in Theorem 6.8.

Hence, condition 1 or condition 2 of Definition 7.4 are satisfied.

- 3. The face H' of G' is a non-trivial L-face. Then one of the following holds:
 - (a) Let l be the only iso-line on H' . Then the following holds:
 - i. H' contains exactly one iso-node and H contains three disperse nodes and one continuous node which is not an iso-node.
 - ii. The iso-line l is common to a pair of iso-paths such that the iso-paths are disperse connected with respect to the common iso-line.

These results follow from Proposition 5.12 and 5.13. Hence, condition 1 of Definition 7.4 is satisfied.

- (b) Let there be an iso-path on H' . Then the following holds:
 - i. There exist three iso-lines on H' .
 - ii. There is one iso-line on H .
 - iii. To each iso-line in H' there exists an iso-path that does not lie on H' .
 - iv. Each iso-line on H' is common to the iso-path on H' and another iso-path that does not lie on H' . Both iso-paths are disperse connected with respect to their common iso-line l .

These results follow from Proposition 5.12 and 5.13. Hence, condition 1 of Definition 7.4 is satisfied.

Case 2: An iso-line $l \in \{l_1, \dots, l_n\}$ lies on a trivial L-face $H(V_h, E_h, \mathcal{F}_h)$ of G .

We consider two subcases.

1. Let H' be a singular or a disperse face of G' .

Then, according to Theorem 6.1 there are two iso-paths in G having l as a common iso-line. These iso-paths are disperse connected with respect to l .

Hence, condition 1 of Definition 7.4 is satisfied.

2. Let H' be a trivial L-face of G' . Then the following holds:

- (a) $H = H'$.
- (b) According to Theorem 6.1 we get two iso-paths in G and two iso-paths in G' and all four iso-paths have the common iso-line l . Then there exists a unique pairing of iso-paths such that the common iso-line l of each pair of iso-paths corresponds to a disperse node of H . Both pairs of iso-paths are then disperse connected with respect to l . But it is not possible that three of them are disperse connected. If this is the case, then there is a disperse path which connects the disperse nodes on H . But for this to happen we need at least five disperse nodes, say in G . Then application of the T_1 -rule to G will change one of the iso-nodes of G on H to a disperse node. But then G has no iso-path that passes through l . Therefore, there cannot exist three iso-paths that pass through l and which are disperse connected.

Hence, condition 2 of Definition 7.4 is satisfied.

Case 3: An iso-line $l \in \{l_1, \dots, l_n\}$ lies on a non-trivial L-face $H(V_h, E_h, \mathcal{F}_h)$ of G .

1. Let there be no iso-path on the L-faces H and H' . Then the following holds:
 - (a) $H' = H$.
 - (b) There exist two iso-lines on H .
 - (c) Each iso-line from (b) is common to a pair of iso-paths which are disperse connected with respect to the common iso-line on H . This follows from Proposition 5.13.

Hence, condition 1 of Definition 7.4 is satisfied.

2. Let there be an iso-path on the L-faces. Then the following holds:

- (a) $H' = H$.
- (b) There exist three iso-lines on H if H has an iso-node; otherwise, there exist four iso-lines on H .

- (c) To each iso-line from (b) there exists an iso-path that does not lie on H .
- (d) Each iso-line from (b) is common to the iso-path on H and another iso-path which does not lie on H . Both iso-paths are disperse connected with respect to the common iso-line l .

These results follow from Proposition 5.12 and 5.13. Hence, condition 1 of Definition 7.4 is satisfied.

□

Based on Theorem 7.5 we give the following definition.

Definition 7.6. (*Disperse connected iso-elements and iso-surface component*). Let the polygonal domain $\Omega \subset \mathbb{R}^3$ have a domain partition $\mathcal{T} = \{C_i\}_{i=1}^N$ into cuboids. Let $\mathcal{G} = \{G_1, \dots, G_N\}$ be a set of labeled cuboid graphs with common iso-level $c \in (0, 1)$, and C_i be the cuboid of G_i for $i = 1, \dots, N$. Assume that all G_i are singular iso-path free and isolated iso-path free. Compute the complete iso-paths in each G_i by applying the algorithm given in Section 5.4. Let the union of all iso-surfaces in \mathcal{G} be denoted by Γ and let Z and \tilde{Z} be two iso-elements in Γ . If there is $r \geq 1$ and if there exist iso-elements Z_0, \dots, Z_r of Γ such that $Z_0 = Z$, $Z_r = \tilde{Z}$ and all pairs (Z_{i-1}, Z_i) , $i = 1, \dots, r$ are neighbored with respect to their common iso-line, then we say Z and \tilde{Z} are disperse connected iso-elements.

We define a component of Γ with respect to an iso-element $Z \subset \Gamma$, denoted by $\Gamma(Z)$, by

- $\Gamma(Z)$ consists of Z and of all iso-elements of Γ which are disperse connected to Z .

Theorem 7.7. (*Connectedness and uniqueness of a component*). An iso-surface component defined as in Definition 7.6 is connected. Furthermore, for any two distinct iso-elements Z_1 and Z_2 of Γ it holds that either $\Gamma(Z_1) = \Gamma(Z_2)$ or $\Gamma(Z_1) \cap \Gamma(Z_2) = \emptyset$ in the sense of convention of iso-elements disjointness. Consequently, the components of Γ are uniquely determined.

Proof. We give the proof in two steps.

1. Uniqueness of components: Note that the relation between iso-elements to be disperse connected is reflexive, symmetric and transitive by its definition. Hence, the set of all iso-elements decomposes into disjoint (in the sense of iso-elements disjointness) equivalence classes, which are precisely the components of Γ . This proves the uniqueness.

2. Connectedness of a component: Let $\Gamma(Z)$ be a component of Γ and let $Z_1, Z_2 \in \Gamma(Z)$ be iso-elements. Then Z_1 is connected to Z and

Z is connected to Z_2 , hence each two iso-elements in $\Gamma(Z)$ are disperse connected. \square

The intersection of two different components is \emptyset in the sense that the intersection does not contain an iso-element, but it may contain discrete points or line segments (cf. *Convention of iso-elements disjointness*). The following remark provides additional information on the intersection of two distinct components of Γ .

Remark 7.8. (*Relations of two distinct components*). We denote from here on the components of Γ by $\Gamma_1, \dots, \Gamma_n$ if Γ has $n \geq 2$ components, where Γ and Γ_i are as in Definition 7.6. Note that the only possibility for two distinct components to have an iso-element in common is if both have a common trivial L-face such that on the L-face there is an iso-element. But such an L-face belongs to only one component, since if there exists an iso-path on the L-face then each iso-line on the L-face is common to only two distinct iso-paths as shown in Proposition 5.13. The first iso-path is the iso-path on the L-face and the second iso-path is an inner iso-path. Therefore, according to Definition 7.6, the iso-path on the L-face belongs to only one component and, hence, all other inner iso-paths which have a common iso-line with the iso-path on the L-face belong to the same component as well. This follows from condition 1 of Definition 7.4.

If two different components have an iso-point or iso-points in common, where none of them are end points of an iso-line for both components, then the common points are vertices of cuboids in the partition \mathcal{T} . In addition, if two different components have an iso-line or iso-lines in common, then the common line segments are edges (cf. Theorem 6.8) or face diagonals (cf. Lemma 6.2) of cuboids in the partition \mathcal{T} . This follows from Definition 7.6 and Theorem 7.7.

8 Surface Normal Vectors and discrete Curvature

For iso-surfaces Γ computed according to the algorithm given in Section 5.4 there exists a decomposition of Γ into components according to Definition 7.6 and Theorem 7.7. By construction, a component is oriented and connected. This section is devoted to solve the following problems:

1. how to compute surface normal vectors of a component,
2. how many iso-points of a component are connected to an iso-point P of the component,
3. constructing an appropriate region in one component around an iso-point P of the component on which discrete mean curvature computation for P is possible.

In this paper we are not giving details on how to compute discrete mean curvature at discrete points of a component since this can be found in the literature (see e.g. [8]), but we show how to identify the required surface region inside a component.

8.1 Surface Normal Vectors

The computation of surface normal vectors of an iso-surface is straight forward, except for determining the same orientation for all iso-surface normal vectors. For all triangles of the triangulated iso-elements, let \mathbf{N} be an arbitrarily oriented surface normal. Then the oriented normal field \mathbf{n} is obtained by choosing $+\mathbf{N}$ or $-\mathbf{N}$, locally. For this purpose we first need to know a direction in which the desired surface normal shall be approximately pointing. We call a vector which approximates the surface normal vector, while giving the same orientation (i.e. angle to \mathbf{n} is below 90°), a *surface pseudo-normal*. Usually, for the computation of such a surface pseudo-normal one needs to know the gradient of the nodal function \mathcal{F} of a labeled cuboid graph $G(V, E, \mathcal{F})$. We give here an alternative method which does not use the gradient of the function \mathcal{F} but instead uses all node positions of G , distinguishing between continuous and disperse nodes.

Let $G(V, E, \mathcal{F})$ be an irreducible labeled cuboid graph with iso-level $c \in (0, 1)$. Let there be $n \geq 3$ iso-points P_i of the iso-path, denoted by ω , in G and let $P_c \in \mathbb{R}^3$ be the center of the iso-element $[P_1, \dots, P_n | P_c]$ corresponding ω . By definition of an iso-surface component as given in Definition 7.6, the orientation of the normal field on an iso-element of G should be pointing towards the continuous nodes of G . Therefore, a surface pseudo-normal for the iso-element, denoted as \mathbf{p} , has to be determined using the position of disperse and continuous nodes of G such that it points from the disperse to the continuous phase. Let \mathbf{N} be a normal of the triangle $\text{Tri}(P_1, P_2, P_c)$, say. Then the surface normal \mathbf{n} on $\text{Tri}(P_1, P_2, P_c)$ is

$$\mathbf{n} = \begin{cases} \mathbf{N} & \text{if } \mathbf{N} \cdot \mathbf{p} > 0 \\ -\mathbf{N} & \text{else.} \end{cases} \quad (38)$$

Remark 8.1. *For iso-surface normal computation, the consideration of irreducible labeled cuboid graphs, is sufficient. First, computation of surface normals of iso-paths which lie on L-faces of a labeled cuboid graph is straight forward. Second, a labeled cuboid graph G can be decomposed into irreducible graphs with respect to inner iso-paths of G as given in (33).*

Surface pseudo-normal: Let $G(V, E, \mathcal{F})$ be an irreducible labeled cuboid graph with iso-level $c \in (0, 1)$. Let $V = \{P_1, \dots, P_8\}$, $N = \{1, 2, \dots, 8\}$ and let N_c and N_d correspond to the set of continuous and disperse node indices of G , respectively. Then $N = N_c \cup N_d$. We compute a surface pseudo-normal

for G by adding all vectors \mathbf{v}_j for $j = 1, \dots, |N_d|$ with \mathbf{v}_j defined by

$$\mathbf{v}_j = \sum_{i \in N_c} (C_i - D_j), \quad j \in N_d, \quad (39)$$

where C_i and D_j are continuous and disperse nodes of G , respectively. Then we get

$$\mathbf{p} = \sum_{j \in N_d} \sum_{i \in N_c} (C_i - D_j) \quad (40)$$

Proposition 8.2. *The surface pseudo-normal vector given in (40) satisfies*

$$\mathbf{p} = |N_d| \sum_{i \in N} P_i - 8 \sum_{j \in N_d} D_j,$$

where $V = \{P_1, \dots, P_8\}$.

Proof. We get the following by using $N = N_c \cup N_d$ and $|N| = 8$:

$$\begin{aligned} \sum_{i \in N_c} (C_i - D_j) &= \sum_{i \in N_c} C_i - |N_c| D_j \\ &= \sum_{i \in N_c} C_i + \sum_{k \in N_d} D_k - |N_c| D_j - \sum_{k \in N_d} D_k \\ &= \sum_{i \in N} P_i - |N_c| D_j - \sum_{k \in N_d} D_k. \end{aligned}$$

By using the above relation we get

$$\begin{aligned} \sum_{j \in N_d} \sum_{i \in N_c} (C_i - D_j) &= \sum_{j \in N_d} \left[\sum_{i \in N} P_i - |N_c| D_j - \sum_{k \in N_d} D_k \right] \\ &= |N_d| \sum_{i \in N} P_i - |N_c| \sum_{j \in N_d} D_j - |N_d| \sum_{k \in N_d} D_k \\ &= |N_d| \sum_{i \in N} P_i - (|N_c| + |N_d|) \sum_{j \in N_d} D_j \\ &= |N_d| \sum_{i \in N} P_i - 8 \sum_{j \in N_d} D_j. \end{aligned}$$

□

8.2 Discrete Curvature

An iso-surface Γ which is computed according to the algorithm given in Section 5.4 is polygonal (piecewise planar). Hence, on a component Γ_0 of Γ only discrete mean curvature computation has a meaning. The discrete mean curvature can be computed on points in Γ_0 which are vertices of the

triangulation of Γ_0 . Any iso-element of Γ is triangulated using a center P_c of the iso-element and its iso-points. Generally, the discrete mean curvature at P_c is nearly zero. Hence, discrete mean curvature computation is mainly important at the iso-points of Γ_0 .

Discrete mean curvature computation methods (see e.g. [8]) use for the computation of discrete mean curvature at an iso-point P of Γ_0 a piece of triangulated surface region around P in which P is contained. This surface region is contained in Γ_0 . Hence, the aim of this section is to compute such a surface region.

The following theorem will give us the minimum and maximum number of neighbors of an iso-point P of Γ_0 such that the neighbors are iso-points in Γ_0 and each of them is incident to P .

Theorem 8.3. *Let $G(V, E, \mathcal{F})$ be a labeled cuboid graph with iso-level $c \in (0, 1)$ and let G be regular. Let Z be an iso-element of G and let the iso-path ω corresponding to Z be given by $\omega = [Q_1, Q_2, \dots, Q_m]$ with $m \geq 3$. We set $r_i = \overline{Q_i Q_{i+1}}$ for $i = 1, \dots, m-1$ and $r_m = \overline{Q_m Q_1}$, which are iso-lines and edges of ω . Let us fix one of the Q_i , say $P := Q_1$. Then there exist $4 \leq n \leq 8$ iso-paths $\omega_1, \dots, \omega_n$ in the system of labeled cuboid graphs of G , where $\omega_1 := \omega$ such that*

1. $l_i = \omega_i \cap \omega_{i+1}$ for $i = 1, \dots, n-1$,

2. $l_n = \omega_n \cap \omega_1$,

with $l_1 = r_1, l_n = r_m$ and

- (i) ω_i and ω_{i+1} are disperse connected with respect to l_i for $i = 1, \dots, n-1$,

- (ii) ω_n and ω_1 are disperse connected with respect to l_n .

This means, if Γ is the iso-surface computed according to the algorithm given in Section 5.4 then all iso-paths $\omega_1, \dots, \omega_n$ belong to the same component $\Gamma(Z)$ of Γ and all these iso-paths have in common the iso-point P and these iso-paths are the only iso-paths in $\Gamma(Z)$ with this property.

Proof. We prove the claim by considering four cases.

Case 1: All faces in the system of graphs of G , where the iso-point P lies, are regular.

In this case the point P is an end point of two iso-lines of ω_1 . Both iso-lines lie in G but on different regular faces. Note that P does not lie on an L-face and hence both regular faces do not each have two disperse and two iso-nodes (according to Lemma 6.4). Hence, on each of these regular faces lies an edge of a unique iso-path according to Proposition 5.12. Therefore, to each neighbor of the faces there exists an iso-path which passes through

an iso-line on the face. Hence, we have two additional iso-paths in two different labeled cuboids. From these two additional iso-paths we get two additional iso-lines with an end point P . Therefore, we get a total of four distinct iso-lines with an end point P . But only three iso-paths cannot give a connected iso-surface at the point P and hence, there exist at least one additional iso-path that passes through P . Hence, there exist $\omega_2, \dots, \omega_4$ satisfying the claim of the proposition which is $n = 4$.

Case 2: The iso-point P is not an iso-node of G and all faces in the system of graphs of G , where the iso-point P lies, are L-faces.

The iso-point P is common to four faces in the system of graphs of G . If each of the L-faces is non-trivial, then on each face we have two iso-lines with end point P . Then we have a total of $n = 8$ iso-lines which are neighbors of P . If some of the L-faces are trivial L-faces, we get $4 \leq n \leq 8$.

Case 3: The iso-point P is an iso-node of G and all faces in the system of graphs of G , where the iso-point P lies, are L-faces.

The iso-point P is common to eight faces in the system of graphs of G . The prove uses the same argument as in Case 1 to get that n is at least four. In case each of the L-faces is non-trivial, we get the same result as in Case 2. In this case, the same argument as in Case 2 can be applied.

Case 4: The iso-point P of G lies on an L-face in the system of graphs of G .

By combining the cases 1, 2 and 3 we then get $4 \leq n \leq 8$. \square

In the next definition, we give the so-called *surface region* Γ_P of an iso-point P within the component Γ_0 of Γ . The surface region Γ_P contains P and all iso-points in Γ_0 which are incident to P . Additionally, Γ_P contains each center of the iso-elements which have P in common. The surface region Γ_P of P can be used to compute discrete mean curvature at P (see e.g. [8]).

Definition 8.4. (*Neighboring iso-lines, iso-points, points and surface region*). Let Z be an iso-element of the iso-surface Γ computed according to the algorithm given in Section 5.4. and let $P \in Z$ an iso-point. Then we call the iso-lines l_1, \dots, l_n which we get from Theorem 8.3 using Z , neighboring iso-lines to P . Then P and l_1, \dots, l_n lie in the component $\Gamma(Z)$. Let the iso-points P_1, \dots, P_n be the other end points of the l_i , i.e. $l_i = \overline{PP_i}$ for $i = 1, \dots, n$. We call P_1, \dots, P_n neighboring iso-points to P . Note that to each iso-line l_i there exists an iso-path ω_i in $\Gamma(Z)$ such that $l_i \subset \omega_i$. All the iso-paths ω_i are different according to Theorem 8.3. Let P_{c_i} be the center of

ω_i and let us denote by $N(\omega_i)$ the number of iso-lines of ω_i . We define

$$\mathcal{E}_i = \begin{cases} \text{Tri}(P, P_i, P_{i+1}) & \text{if } N(\omega_i) = 3 \text{ or } \omega_i \text{ is an outer iso-path} \\ \text{Tri}(P, P_i, P_{c_i}) \cup \text{Tri}(P, P_{i+1}, P_{c_{i+1}}) & \text{else} \end{cases}$$

for $i = 1, \dots, n-1$, and

$$\mathcal{E}_n = \begin{cases} \text{Tri}(P, P_n, P_1) & \text{if } N(\omega_n) = 3 \text{ or } \omega_n \text{ is an outer iso-path} \\ \text{Tri}(P, P_n, P_{c_n}) \cup \text{Tri}(P, P_1, P_{c_1}) & \text{else.} \end{cases}$$

We then call the piece of iso-surface Γ_P defined by

$$\Gamma_P := \cup_{i=1}^n \mathcal{E}_i$$

the surface region of P . In addition, we define a set of points \mathcal{P}_i by

$$\mathcal{P}_i = \begin{cases} \{P_i, P_{i+1}\} & \text{if } N(\omega_i) = 3 \text{ or } \omega_i \text{ is an outer iso-path} \\ \{P_i, P_{c_i}, P_{i+1}, P_{c_{i+1}}\} & \text{else} \end{cases}$$

for $i = 1, \dots, n-1$, and

$$\mathcal{P}_n = \begin{cases} \{P_n, P_1\} & \text{if } N(\omega_n) = 3 \text{ or } \omega_n \text{ is an outer iso-path} \\ \{P_n, P_{c_n}, P_1, P_{c_1}\} & \text{else.} \end{cases}$$

Finally, we set $\mathcal{D}_P := \cup_{i=1}^n \mathcal{P}_i$.

Computation of discrete mean curvature: Let Γ_P and P be as defined in Definition 8.4. The discrete mean curvature at the iso-point P is computed by integrating $\Delta_\Gamma \mathbf{x}$ over Γ_P , where Δ_Γ denotes the Laplace-Beltrami operator. The surface Γ_P is piecewise linear. Therefore, we can give nodal functions defined on Γ_P with values 1 on one of the points $\{P\} \cup \mathcal{D}_P$ and zero on the other points, where \mathcal{D}_P is computed according to Definition 8.4. Applying these nodal functions as a basis for \mathbf{x} and using Gauss's theorem for surface integration of $\Delta_\Gamma \mathbf{x}$ over Γ_P we get the discrete mean curvature at the iso-point P . For more details on this computation of discrete mean curvature see [8].

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